SOME STUDIES OF THE THEORY AND APPLICATION OF CONTINUOUS GROUPS IN ATOMIC SPECTROSCOPY

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To my Wife

with thanks for her encouragement

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ABSTRACT

This thesis is concerned with the representation theory of continuous groups both compact and non-compact and its application to atomic spectroscopy. In Chapter I some atomic wavefunctions for equivalent electrons in the group scheme $SU_2 \times (U_{2\ell+1} \supset R_{2\ell+1} \supset R_3)$ are constructed in terms of electron fermion creation and annihilation operators. The concept of semiconjugacy is defined and shown to reduce the number of states that must be explicitly calculated. The states of the d shell are calculated and tabulated. In Chapter II it is shown how to extract n-body cfp's associated with arbitrary auxiliary quantum numbers from the n-body generalisation of Redmond's formula. The method is applied to give explicit formulae for the squares of one body cfp's of the atomic d-shell.

Group theory is applied in Chapter III to extend the quasiparticle formalism developed by Armstrong and Judd to expose the complete group structure of the eigenfunctions of the equivalent electron ℓ shell. A simple method for relating quasiparticle states to determinantal states and for calculating quasiparticle matrix elements is developed. The need for fractional parentage coefficients in calculating these matrix elements is eliminated. In Chapter IV the

technique and formalism is extended to describe general mixed configurations.

The hydrogen atom is factorised according to the scheme $O(4,2) \supset O(2,1) \times O(3)$ in Chapter V and the radial group $O(2,1)$ studied. It is shown that $r^k D_{\frac{n}{n+q}}$, where D_a is a dilatation operator, is proportional to a tensor operator in this scheme, allowing a group theoretical study of the radial matrix element r^k, including an explanation of the Pasternack and Sternheimer selection rule. The technique is extended in Chapter VI to solve a differential equation directly related to the generalised Kepler equation of Infeld and Hull in an $O(2,1) \times O(3)$ group scheme. This equation contains as special cases the Schrodinger, Klein-Gordan, and Dirac (two forms) hydrogen atoms. A generalised Pasternack and Sternheimer selection rule exists and some matrix elements can be evaluated group theoretically.

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SECTION II - APPLICATIONS

INTRODUCTION

This thesis is concerned with the representation theory of continuous groups and its application to atomic spectroscopy. The use of compact groups to label n particle states and to simplify the computation of matrix elements was pioneered by Racah[1]. To successfully use this technique one requires an extensive knowledge of Kronecker products, branching rules, and coupling or Clebsch-Gordan coefficients of the groups one is using. An extensive literature has been built up over the years relating to these topics. Access to this literature can be gained through the following review papers:
"Group Theory and Spectroscopy" by G. Racah[2],
"Group Theory in Atomic Spectroscopy" by B.R. Judd[3],
"Recent Progress Toward a Theory of Tensor Operators in the Unitary Groups" by J.D. Louck[4], and from the texts of B.R. Judd[5,6] "Operator Techniques in Atomic Spectroscopy" and "Second Quantization and Atomic Spectroscopy" and B.G. Wybourne[7] "Symmetry Principles and Atomic Spectroscopy".

Very recently non-compact groups have been applied to atomic spectroscopy[8-10], in particular the O(4,2) model of the hydrogen atom due to Barut and Kleinert[8]. So recent has been this appearance that to date only the one electron problem has been treated. It would seem that the application

of non-compact groups to the many electron problem is the direction in which atomic spectroscopy is heading.

My thesis is divided into two sections: Section I, Theory, Section II, Application. Section I is concerned with some aspects of the mechanics of compact representation theory, in particular fractional parentage coefficients (cfp's) - special cases of coupling coefficients. In detail in Chapter I I show how to construct fermion wavefunctions for equivalent ℓ electrons with definite unitary ($U(2\ell+1)$) and rotational ($R(2\ell+1)$) symmetry[11]. Special cases containing also $R(3)$ symmetry are constructed. I define the concept of semiconjugacy and show that it reduces the number of states that must be explicitly calculated. For d electrons all possible $R(3)$ states are constructed. Chapter II contains a refinement to Redmond's method for calculating cfp's that enables me to give closed (if somewhat complex) formulas for the square of all cfp's for d electrons.

Section II is concerned with the application of continuous groups, both compact and non-compact, to atomic spectroscopy. Chapter III extends a new method of classifying electron wave functions initially developed by Armstrong and Judd[12,13]. This technique has the advantages that it provides a rich classificatory scheme (it distinguishes all states with the same spin (S) and orbital

angular momentum (L) quantum numbers up to $\ell = 3$, and for $\ell > 4$ is much more successful than the usual classification schemes) and that it allows general operator-matrix-element evaluation without the use of cfp's. Its disadvantage is that spin and particle number quantum numbers are lost. This so called quasiparticle formalism is extended to inequivalent electrons[14] in Chapter IV.

In Chapter V the non-compact group O(2,1) is used to examine the radial eigenfunctions of the hydrogen atom. Armstrong[9] has used this group but his approach does not fit into an embracing group scheme like the O(4,2) model of the hydrogen atom due to Barut and Kleinert[8] that I use in this thesis. The use of O(2,1) enables one to find a selection rule on radial matrix elements discovered by Pasternack and Sternheimer[15] in 1962. One can then evaluate matrix elements diagonal in the principle quantum number n by use of the Wigner-Eckart theorem. In the final chapter of this thesis this technique is extended to a generalised Kepler problem allowing me to deal simultaneously with the hydrogen atoms of Schrodinger, Klein-Gordan and Dirac (two forms).

SECTION I

THEORY

C H A P T E R I

SECOND QUANTIZED ATOMIC WAVEFUNCTIONS WITH DEFINITE UNITARY AND ROTATIONAL SYMMETRY[11]

1. Introduction

It has been known for some time[15-18] that the bases for the irreducible representations of the classical groups can be constructed in terms of sums of products of boson creation and annihilation operators acting on a suitably defined vacuum. The group U_n has been extensively studied using the canonical chain $U_n \supset U_{n-1} \supset \ldots \supset U_1$ as the solution to the state labelling problem[17,18]. SU_3 has also been investigated by this technique using the scheme $SU_3 \supset R_3$[17,19].

Moshinsky[20] has shown that the same analysis can be repeated using fermion operators. Using this method J. Flores et al.[21] analysed the group U_6 in the scheme $U_6 \supset R_6 \supset R_5 \supset R_3$ for all representations of U_6 of the form $\{4^a 3^b 2^c 1^d\}$, i.e. for nucleons, while in this chapter, I identify the fermion creation operator as a single electron creation operator with orbital angular momentum

ℓ and spin of $\frac{1}{2}$, and using the scheme widely used by atomic spectroscopists for a configuration of equivalent electrons[1,5] viz. $SU_2 \times (U_{2\ell+1} \supset R_{2\ell+1} \supset R_3)$ construct some of the basis states for the representations $\{2^a 1^b\}$, $S = \frac{1}{2}b$ (S is the total spin quantum number) of the group $SU_2 \times U_{2\ell+1}$ in terms of sums of products of single electron wavefunctions.

The method used to construct these states is essentially one of projection with the Casimir operator at the $R_{2\ell+1}$ level, coupled with the demand at the R_3 level that L_+ and S_+ on the state be zero (Section 3). Hence, unless otherwise stated, every state in this Chapter has $M_L = L$ and $M_S = S = \frac{1}{2}b$. Lower states can of course be derived by stepping down with L_- and S_-. This differs from the technique of Flores et al. which demands the raising operators of $R_{2\ell+1}$ on the state be zero and then obtains the R_3 state by the use of a lowering operator. This method exploits the inherent greater simplicity of the atomic wavefunctions over nuclear wavefunctions, so that an explicit closed formula can be given for the states $|\{2^a 1^b\}[2^c 1^d]L_M\rangle$ where L_M is the maximum value of L in the branching rule for the $[2^c 1^d]$ representation of $R_{2\ell+1}$ upon being restricted to R_3. Closed formulae can also be given for some $R_{2\ell+1}$ representations for all values of L, viz. [0], [1], [11] and [2].

In Section 5 the concept of semiconjugacy is defined, which, together with some group theory, allows any state to be written down once the state $|\{2^c 1^d\}[2^c 1^d]L\rangle$ is known. In Section 6 the preceding theory is illustrated by calculating and tabulating the wavefunctions for the multiplicity free case of the d shell.

2. Group Generators

Judd[5] has shown that the generators of the group $U_{2\ell+1}$ are

$$X_{ab} = \sum_{k,q} (-1)^{\ell-a} [k]^{\frac{1}{2}} \begin{pmatrix} \ell & k & \ell \\ -a & q & b \end{pmatrix} V^{(k)}_q$$

while the generators of the group $R_{2\ell+1}$ are

$$W_{ab} = \sum_{k,q} (-1)^{\ell-a} (1-(-1)^k) [k]^{\frac{1}{2}} \begin{pmatrix} \ell & k & \ell \\ -a & q & b \end{pmatrix} V^{(k)}_q$$

If we substitute for $V^{(k)}_q$ using the formula[6]

$$W^{(Kk)}_{\pi q} = -\tfrac{1}{2} (\underline{a}^\dagger \underline{a})^{(Kk)}_{\pi q}$$

these become

$$X_{ab} = \sum_{m_s} a^\dagger_{m_s,a} a_{m_s,b}$$

and

$$W_{ab} = \sum_{m_s} (a^{\dagger}_{m_s,a}\, a_{m_s,b} - (-1)^{a+b}\, a^{\dagger}_{m_s,-b}\, a_{m_s,-a})$$

$$= X_{ab} - (-1)^{a+b}\, X_{-b-a} \qquad \text{(I-1)}$$

where the a's are single electron creation or annihilation operators, with subscripts identifying respectively spin and orbital angular momentum projections. These operators are just proportional to Moshinsky's[20] C^b_a and Λ^b_a respectively, in fact $X_{ab} = C^b_a$ and $\Lambda^b_a = \frac{1}{2}W_{ab}$.

If I invert the expression for the $U_{2\ell+1}$ generators I get

$$V^{(k)}_q = \sum_{a,b} (-1)^{\ell-a}[k]^{\frac{1}{2}} \begin{pmatrix} \ell & k & \ell \\ -a & q & b \end{pmatrix} X_{ab}$$

by noting that[15]

$$\underline{V}^{(1)} = \underline{L}[3/\ell(\ell+1)(2\ell+1)]^{\frac{1}{2}}$$

I have that the R_3 generators, i.e. the components of the vector $\underline{L}$, are given by

$$\underline{L} = [\ell(\ell+1)(2\ell+1)]^{\frac{1}{2}} \sum_b (-1)^{\ell-b} \begin{pmatrix} \ell & 1 & \ell \\ -b & q & b-q \end{pmatrix} X_{b\ b-q}$$

$$= \sum_b t^q_b\, X_{q\ b-q} \qquad \text{(I-2)}$$

where $t^q_b = (-1)^{\ell-b}[\ell(\ell+1)(2\ell+1)]^{\frac{1}{2}} \begin{pmatrix} \ell & 1 & \ell \\ -b & q & b-q \end{pmatrix}$

Note that $t^q_b = t^q_{q-b}$.

The generators for the group SU_2, namely $S_{\pm 1}$ and S_0 are given by $\underline{S} = [2\ell+1/2]^{\frac{1}{2}}\underline{W}^{(10)}$ so for instance S_{+1} in second quantized form becomes

$$S_{+1} = + \frac{1}{\sqrt{2}} \sum_{m_\ell} a^\dagger_{\frac{1}{2}m_\ell} a_{-\frac{1}{2}m_\ell}$$

If we now define

$$\nabla^{\frac{1}{2}}_{a_1..a_n} \nabla^{-\frac{1}{2}}_{b_1..b_m} = a^\dagger_{\frac{1}{2}a_1}.. a^\dagger_{\frac{1}{2}a_n} \; a^\dagger_{-\frac{1}{2}b_1}.. a^\dagger_{-\frac{1}{2}b_m}$$

a somewhat specialized form of Moshinsky's[17,20] ∇, then it follows immediately from definitions that

$$X_{ab} \nabla^{\frac{1}{2}}_{\mu_1..\mu_n} \nabla^{-\frac{1}{2}}_{\nu_1..\nu_m}$$

$$= \delta(\mu_i,b)\nabla^{\frac{1}{2}}_{\mu_1..\mu_{i-1}\, a\, \mu_{i+1}..\mu_n} \nabla^{-\frac{1}{2}}_{\nu_1..\nu_m}$$

$$+ \delta(\nu_i,b)\nabla^{\frac{1}{2}}_{\mu_1..\mu_n} \nabla^{-\frac{1}{2}}_{\nu_1..\nu_{i-1}\, a\, \nu_{i+1}..\nu_m} \qquad \text{(I-3)}$$

and

$$S_{+1}\nabla^{\frac{1}{2}}_{\mu_1..\mu_n} \nabla^{-\frac{1}{2}}_{\nu_1..\nu_m}$$

$$= + \frac{1}{\sqrt{2}} \sum_i (-1)^i \nabla^{\frac{1}{2}}_{\mu_1..\mu_n\, \nu_i} \nabla^{-\frac{1}{2}}_{\nu_1..\nu_{i-1}\, \nu_{i+1}..\nu_m} \qquad \text{(I-4)}$$

3. Rotational Symmetry

The condition on the form of the state is found in this section in order that it transform according to definite $U_{2\ell+1}$, $R_{2\ell+1}$ and R_3 symmetry. Clearly

$$\mathcal{U} = \nabla^{\frac{1}{2}}_{\ell\ \ell-1..\ell-a-b+1}\ \nabla^{-\frac{1}{2}}_{\ell\ \ell-1..\ell-a+1}$$

is the greatest weight state of $\{2^a1^b\}$, $S = \frac{1}{2}b$ for $SU_2 \times U_{2\ell+1}$ since $X_{\mu\nu} = 0$, $\mu > \nu$ and $S_{+1} = 0$ while $X_{ii} = k$ where $k = 2$, 1 or 0 if $\ell-a+1 < i < \ell$, $\ell-a-b+1 < i < \ell-a$ or $i < \ell-a-b$ respectively, while $S_0 = \frac{1}{2}b$. By application of the step down operators of $U_{2\ell+1}$, namely $X_{\mu\nu}$, $\mu < \nu$, it can be seen that a state of arbitrary weight of the representation $\{2^a1^b\}$ of $U_{2\ell+1}$ (but of maximum weight in SU_2) takes the form of a linear combination of states like $\nabla^{\frac{1}{2}}_{\mu_1..\mu_{a+b}}\ \nabla^{-\frac{1}{2}}_{\nu_1..\nu_a}$. To apply the additional constraint that this state $|T\rangle$ transforms according to the representation $[2^c1^d]$ of $R_{2\ell+1}$ we demand that

$$G|T\rangle = g|T\rangle \qquad \text{(I-5)}$$

where G is the Casimir operator of $R_{2\ell+1}$ having the eigenvalue g for the representation $[2^c1^d]$.

The Casimir operator for $R_{2\ell+1}$ is[5]

$$G = \sum_{a,b} W_{ab}W_{ba}$$

which, following Moshinsky[20], we write as (from equation (I-1))

$$\sum_{a,b}(X_{ab} - (-1)^{a+b}X_{-b-a})(X_{ba} - (-1)^{a+b}X_{-a-b})$$

$$= 2\sum_{a,b}X_{ab}X_{ba} - 2\sum_{a,b}(-1)^{a+b}X_{ab}X_{-a-b}.$$

$$\text{i.e.} \quad G = 2\Gamma - 2\rho \tag{I-6}$$

where $\rho = \sum_{a,b}(-1)^{a+b}X_{ab}X_{-a-b}$, and Γ is the Casimir operator for $U_{2\ell+1}$. The eigenvalues of Γ acting on a state that transforms according to $\{2^a1^b\}$ can be found by operating Γ on the greatest weight state of $\{2^a1^b\}$ giving

$$\Gamma\nabla^{\frac{1}{2}}_{\ell\ \ell-1..\ell-a-b+1}\nabla^{-\frac{1}{2}}_{\ell\ \ell-1..\ell-a+1}$$

$$= [(2\ell+2-a-b)(a+b) + (2\ell+4-a)a]^{\frac{1}{2}}\nabla^{\frac{1}{2}}_{\ell\ \ell-1..\ell-a-b+1}\nabla^{-\frac{1}{2}}_{\ell\ \ell-1..\ell-a+1} \tag{I-7}$$

while the eigenvalues of G for the representation $[2^c1^d]$ of $R_{2\ell+1}$ are found by substitution in the formula $2\sum_{i=1}^{\ell}w_i(w_i+1+2\ell-2i)$ given by Judd[5] for the representation $[w_1..w_\ell]$ of $R_{2\ell+1}$. The result is $4c(2\ell+2-c)+2d(2\ell+1-2c-d)$. The $R_{2\ell+1}$ condition, equation (I-5), taken with (I-6) and (I-7) thus becomes

$$|T\rangle = [(a+b)(2\ell+2-a-b) + a(2\ell+4-a) - 2c(2\ell+2-c)$$

$$-d(2\ell+1-2c-d)]|T\rangle$$

$$= p|T\rangle \qquad \text{(I-8)}$$

We examine first then the action of on a general mononomial state $S = \nabla^{\frac{1}{2}}_{\mu_1 \cdots \mu_{a+b}} \nabla^{-\frac{1}{2}}_{\nu_1 \cdots \nu_a}$. We write ρ as

$$= \sum_{a\neq 0} X_{-a-a}X_{aa} + \sum_{a\neq 0} X_{a-a}X_{-aa} + \sum_{\substack{a,b \\ a\neq \pm b}} (-1)^{a+b} X_{-b-a}X_{ba} + X_{00}X_{00}$$

$$= \sum_{a>0} (X_{-a-a}X_{aa} + X_{aa}X_{-a-a}) + \sum_{a>0} (X_{a-a}X_{-aa} + X_{-aa}X_{a-a})$$

$$+ \sum_{\substack{b \\ b\neq \pm a}} \left(\sum_{a>0} (-1)^{a+b} [X_{-b-a}X_{ba} + X_{-ba}X_{b-a}] \right) + \sum_{\substack{b \\ b\neq 0}} (-1)^{b} X_{-b0}X_{b0}$$

$$+ X_{00}X_{00}$$

and look at each term in turn.

1. $X_{-a-a}X_{aa} + X_{aa}X_{-a-a}$. Effective only if both $\pm a$ present in S. Gives an eigenvalue of $2N_aN_{-a}$ where $N_{\pm a}$ is the number of $\pm a$'s present in S.

2. $X_{a-a}X_{-aa} + X_{-aa}X_{a-a}$. Effective if S contains a or $-a$, or both if they are present in opposite spin spaces. Gives an eigenvalue $(N^{\uparrow}_a - N^{\uparrow}_{-a})^2 + (N^{\downarrow}_a - N^{\downarrow}_{-a})^2$ where the superscripted arrows specify in which spin space we are counting

the ±a's. Gives also a term of the form (i.e. other orbital angular momentum projection quentum numbers m_ℓ, may also be present in the state, distributed in an arbitrary manner), $2\nabla^{\frac{1}{2}}_{..-a..}\ \nabla^{-\frac{1}{2}}_{..a..}$ if S is of the form $\nabla^{\frac{1}{2}}_{..a..}\ \nabla^{-\frac{1}{2}}_{..-a..}$.

3. $\sum_{\substack{b \\ b\neq\pm a}} (-1)^{a+b}(X_{-b-a}X_{ba}+X_{-ba}X_{b-a})$. Effective only if S contains both ±a. However, if they are both present in the same spin space we have

$$\sum_{\substack{b \\ b\neq\pm a}} (-1)^{a+b}(X_{-b-a}X_{ba}+X_{-ba}X_{b-a})\nabla^{\pm\frac{1}{2}}_{..a\mu_1..\mu_k-a..}$$

$$= \sum_{\substack{b \\ b\neq\pm a}} (-1)^{a+b}(\nabla^{\pm\frac{1}{2}}_{..b\mu_1..\mu_k-b..} + \nabla^{\pm\frac{1}{2}}_{..-b\mu_1..\mu_k b..})$$

$$= \sum_{\substack{b \\ b\neq\pm a}} (-1)^{a+b}(\nabla^{\pm\frac{1}{2}}_{..b\mu_1..\mu_k-b..}[1+(-1)^{k+k-1}])$$

$$= 0.$$

So a term of the form $\nabla^{\frac{1}{2}}_{..a..}\ \nabla^{-\frac{1}{2}}_{..-a..}$ becomes

$$2\sum_{\substack{b \\ b\neq\pm a}} (-1)^{a+b}\nabla^{\frac{1}{2}}_{..b..}\ \nabla^{-\frac{1}{2}}_{..-b..}.$$

4. $\sum_{\substack{b \\ b\neq 0}} X_{-b0}X_{b0}$. Effective only if S is of the form $\nabla^{\frac{1}{2}}_{..0..}\nabla^{-\frac{1}{2}}_{..0..}$. S becomes $2\sum_{\substack{b \\ b\neq 0}} (-1)^b \nabla^{\frac{1}{2}}_{..b..}\nabla^{-\frac{1}{2}}_{..-b..}$.

5. $X_{00}X_{00}$. Effective if S contains zeros giving an eigenvalue of N_0^2.

Hence

$$\rho S = \sum_{a>0} [N_0^2 + 2N_a N_{-a} + (N_a^{\uparrow} - N_{-a}^{\uparrow})^2 + (N_a^{\downarrow} - N_{-a}^{\downarrow})^2]S \qquad \text{(I-9)}$$

from 1, 2 and 5, <u>plus</u> terms in which each external a, -a pair, (i.e. a and -a in different spin spaces) is replaced by a sum through an external b, -b pair, for all $b \neq a$, this term being derived from 2, 3 and 4. This term will be written as

$$\delta(P^{\uparrow\downarrow}>0)2 \sum_{\substack{\text{each} \\ \text{pair}}} \sum_{b\neq a} (-1)^{a+b} \nabla^{\frac{1}{2}}_{..b..}\nabla^{-\frac{1}{2}}_{..-b..} \qquad \text{(I-10)}$$

where $P^{\uparrow\downarrow}$ is the number of external pairs in S and $\delta(P^{\uparrow\downarrow}>0)$ signifies that this term exists only if there is at least one external pair. The first term (I-9) can be further simplified for, using the notation that $P^{\uparrow}(P^{\downarrow})$ is the number of internal pairs in the spin up (down) space, while $^{\uparrow}(\ ^{\downarrow})$ is the total number of electrons in the spin up (down) space we have

$$\sum_a 2N_aN_{-a} = 2(P^{\uparrow}+P^{\downarrow}+P^{\uparrow\downarrow}-\tfrac{1}{2}N_0(N_0-1)) \qquad \text{(I-11a)}$$

and

$$\sum_{a>0}(N_a^{\uparrow}-N_{-a}^{\uparrow})^2 = \mathcal{L}^{\uparrow} - 2P^{\uparrow} - N_0^{\uparrow} \qquad \text{(I-11b)}$$

and similarly for spin down. Since $\mathcal{L}^{\uparrow}+\mathcal{L}^{\downarrow}$ equals the total number of electrons, equals 2a+b, we have by (I-11) that

$$\sum_{a>0}[N_0^2+2N_aN_{-a} + (N_a^{\uparrow}-N_{-a}^{\uparrow})^2 + (N_a^{\downarrow}-N_{-a}^{\downarrow})^2] = 2a+b+2P^{\uparrow\downarrow} \qquad \text{(I-12)}$$

In all then ((I-10) and (I-12))

$$\mathcal{P}S = (2a+b+2P^{\uparrow\downarrow})S + \delta(P^{\uparrow\downarrow}>0)2 \sum_{\substack{\text{each}\\ \text{pair}}} \sum_{b\neq a} (-1)^{a+b} \nabla_{\frac{1}{2}}^{\frac{1}{2}} \nabla_{..b..}^{-\frac{1}{2}} \nabla_{..-b..}^{-\frac{1}{2}} \qquad \text{(I-13)}$$

Returning now to the $R_{2\ell+1}$ condition (I-8) and writing $|T\rangle$ as

$$|T\rangle = \sum_S \alpha_S S$$

where S is of the mononomial form as used above and α_S are unknown coefficients to be determined, we have immediately that

$$p\alpha_S = (2+b+2P_S^{\uparrow\downarrow})\alpha_S + \delta(P_S^{\uparrow\downarrow}>0)2 \sum_{\substack{\text{each}\\ \text{pair}}} \sum_{b\neq a} (-1)^{a+b} \alpha \nabla_{\frac{1}{2}}^{\frac{1}{2}} \nabla_{..b..}^{-\frac{1}{2}} \nabla_{..-b.}^{-\frac{1}{2}} \qquad \text{(I-14)}$$

where the subscript to the P indicates that the pair

counting is being taken over the state S. If we now form the matrix array A of coefficients of a_S for all S, which will have $2a+b+2P_S^{\uparrow\downarrow}$ as diagonal elements and ± 2 as non-diagonal elements (remembering that terms like $\nabla^{\frac{1}{2}}_{..a..b..}$ $\nabla^{-\frac{1}{2}}_{..-a..-b..}$ and $\nabla^{\frac{1}{2}}_{..b..a..}$ $\nabla^{-\frac{1}{2}}_{..-b..-a..}$ are equal so their ± 2 coefficient will appear in the same column) then the $R_{2\ell+1}$ condition (I-14) becomes:- if the eigenvalues of matrix A are equal to p then the corresponding eigenstate transforms according to $\{2^a 1^b\}[2^c 1^d]$ of $U_{2\ell+1}$ and $R_{2\ell+1}$. We note that several distinct values of p may satisfy this condition.

Moreover we see that if S has n external pairs then each term in the above equation (I-14) has n external pairs; thus A breaks up into block diagonal form, each block associated with a different number of (external) pairs. The problem thus reduces to finding the eigenvalues and eigenstates for each block separately.

Finally the R_3 and SU_2 greatest weight condition is imposed by demanding that $L_{+1} = \sum_b t^q_b X_{q\ b-q}$ (I-2) and S_{+1} on the state be zero, giving a set of simultaneous equations, which in the general case will have a set of solutions corresponding to the multiplicity of L in the branching rule of $[2^c 1^d]$ upon restriction to R_3. If at any stage in the $U_{2\ell+1} \supset R_{2\ell+1} \supset R_3$ chain one attempts to construct a

state forbidden by the corresponding branching rule, one will get a vanishing result.

The R_2 condition that the state has a definite M_L (equal to L in our case) is simply fulfilled by demanding that each mononomial of type S in the state has the sum of its m_ℓ quantum numbers equal to M_L.

4. Some Generalities

The eigenvalues and eigenvectors for matrix A have been found for the zero and one pair case, together with one important solution for the n pair case. Before deriving these, we will first examine the $U_{2\ell+1} \rightarrow R_{2\ell+1}$ branching rules. These can be divided into two classes[5,23,24], namely

$$1.\quad a+b < \ell,\ \{2^a 1^b\} \rightarrow \sum_{x=0}^{a} [2^{a-x} 1^b] \qquad \text{(I-15a)}$$

$$2.\quad a+b > \ell,\ \{2^a 1^b\} \rightarrow \sum_{x=0}^{\mathrm{Min}(a,a+b-\ell-1)} [2^{a-x} 1^{2+1-2a-b+2x}]$$

$$+ \sum_{x=a+b-\ell}^{a} [2^{a-x} 1^b] \qquad \text{(I-15b)}$$

In all the above cases it is assumed that $2a+b < 2\ell+1$. States with $2a+b > 2\ell+1$ can be found by utilizing the particle-hole equivalence[1,5]. p thus takes two different forms ((I-15a) and the first term in (I-15b))

the relation between a and b, and c and d being different in each case. Upon substitution into the formula for p (I-8) we get in each case

1. $p = 4x\ell+2x(x+2)+2(1-2x)a+(1-2x)b.$

2. As for 1. (but not trivially so).

We consider now the function

$$F_m = \sum_{\mu_1>\mu_2>\cdots>\mu_m} (-1)^{\mu_1+\mu_2+\cdots+\mu_m} \nabla^{\frac{1}{2}}_{q_1 q_2 \cdots q_{c'+d'} \mu_1 \mu_2 \cdots \mu_m} \times \nabla^{-\frac{1}{2}}_{r_1 r_2 \cdots r_{c'} -\mu_1 -\mu_2 \cdots -\mu_m} \qquad \text{(I-16)}$$

which has

$$\alpha \; \nabla^{\frac{1}{2}}_{q_1 \cdots q_{c'+d'} \mu_1 \cdots \mu_m} \; \nabla^{-\frac{1}{2}}_{r_1 \cdots r_{c'} -\mu_1 \cdots -\mu_m} = (-1)^{\mu_1+\mu_2+\cdots\mu_m}$$

$m = a-c'$ where c' and d' are the values of c and d before Murnaghan's[24] modification rules have been applied, that is, $c' = a-x$ and $d' = b$. $\mu_1, \mu_2, \cdots \mu_m$ are summed through all permissible values, their ordering being simply to avoid a redundancy of states as mentioned in Section 3. If we substitute these values for α in matrix A (I-14), we get the expression

$$(2a+b+2m)(-1)^{\mu_1+\cdots+\mu_m}$$

$$+ 2\sum_{i=1}^{m} \sum_{\nu_i \neq \mu_i} (-1)^{\mu_i+\nu_i}\cdot(-1)^{\mu_1+\cdots+\mu_{i-1}+\nu_i+\mu_{i+1}+\cdots+\mu_m}$$

$$= (-1)^{\mu_1+\cdots+\mu_m}\left[2a+b+2m+2\sum_{i=1}^{m} \sum_{\nu_i \neq \mu_i} 1\right] \qquad \text{(I-17)}$$

By inspection of the values ν_i can take in the expression $\nabla^{\frac{1}{2}}_{q_1\cdots q_{c'+d'}\mu_1\cdots\mu_m} \nabla^{-\frac{1}{2}}_{r_1\cdots r_{c'}\,-\mu_1\cdots-\mu_m}$ we find that

$$\sum_{\nu_i \neq \mu_i} 1 = 2\ell+1-a-b-c'.$$

Hence (I-17) becomes $4m\ell+4m+2(1-m)a + (1-2m)b-2mc'$. As we vary c' through case 1 and 2 (I-15) above we find quite remarkably that this expression equals the corresponding expression for p with m in place of x. Thus the $R_{2\ell+1}$ condition (I-14) is satisfied, establishing that F_m (I-16) transforms according to $\{2^a 1^b\}[2^{a-m} 1^b]$ or $\{2^a 1^b\}[2^{a-m} 1^{2\ell+1-2a-b+2m}]$ according to the relative sizes of a, b and m. Clearly F_m reduces to just one term if m = 0, so all non-paired mononomials transform according to $\{2^a 1^b\}[2^a 1^b]$ or $\{2^a 1^b\}[2^a 1^{2\ell+1-2a-b}]$. We can find a second eigenstate of the submatrix of A associated with m = 1 by letting x = 0. This gives as a solution the single pair identity

$$\sum_{\text{All } a} (-1)^a \alpha \, \nabla^{\frac{1}{2}}_{..a} \nabla^{-\frac{1}{2}}_{..-a} = 0 \qquad \text{(I-18)}$$

In brief then, the submatrix associated with m = 0, gives as its complete set of solutions mononomials transforming according to the pair of $U_{2\ell+1}$ and $R_{2\ell+1}$ representations associated with x = 0, which we shall shorten to - transforming as x = 0. The n×n matrix associated with m = 1 gives a one dimensional solution F_1, transforming as x = 1, and an n-1 dimensional solution (I-18) transforming as x = 0. Clearly A is symmetric, hence all possible one pair solutions have been exhausted. For a general number of pairs I have been able to find only a one dimensional solution F_m (I-16), transforming as x = m.

The state $|\{2^a 1^b\}[2^c 1^d] L_M\rangle$ where L_M is the maximum L in the $R_{2\ell+1} \rightarrow R_3$ branching rule for $[2^c 1^d]$ can now be written down as

$$\mathcal{J}_m = N \sum_{\mu_1>\mu_2>..>\mu_m} (-1)^{\mu_1+\mu_2+..\mu_m} \nabla^{\frac{1}{2}}_{\ell\, \ell-1..\ell-c'-d'+1\, \mu_1\mu_2..\mu_m}$$

$$\times \nabla^{-\frac{1}{2}}_{\ell\, \ell-1..\ell-c'+1-\mu_1..-\mu_m} \qquad \text{(I-19)}$$

where m = a-c' as before and N is a normalisation constant. This is so since the state satisfies the $U_{2\ell+1}$ and $R_{2\ell+1}$ conditions, has $M_L = L$, $M_S = S = \frac{1}{2}b$ and

$$L_{+1}\mathcal{J}_m = \left(\sum_{a=c+d-\ell-1}^{\ell-c+1} t_a^1 \, X_{a\ a-1}\right)\mathcal{J}_m$$

$$= N \sum_i \Bigg(\sum_{\mu_1>..>\mu_{i-1}>\mu_i+1,\, \mu_i>\mu_{i+1}\mu..>\mu_m} t^1_{\mu_{i+1}}$$

$$\times \nabla^{\frac{1}{2}}_{\ell..\ell-c'-d'+1\ \mu_1..\mu_{i-1}\mu_i+1\mu_{i+1}..\mu_m}\ \nabla^{-\frac{1}{2}}_{\ell..\ell-c'+1-\mu_1..-\mu_m}$$

$$\overset{+}{\mu_1}>..>\mu_{i-1}>\mu_i, \sum_{\mu_i-1>\mu_{i+1}>..>\mu_m} t^1_{-\mu_i+1}$$

$$\times \nabla^{\frac{1}{2}}_{\ell..\ell-c'-d'+1\ \mu_1..\mu_m}\ \nabla^{-\frac{1}{2}}_{\ell..\ell-c'+1-\mu_1..-\mu_{i-1}-\mu_i+1\ \mu_{i+1}..\mu_m}\Bigg)$$

$$= N \sum_i \sum_{\mu_1>..>\mu_{i-1}>\mu_i, \mu_i-1>\mu_{i+1}>..>\mu_m} t^1_{\mu_i}((-1)^1+1)$$

$$\times\ \nabla^{\frac{1}{2}}_{\ell..\ell-c'-d'+1\ \mu_1..\mu_m}\ \nabla^{-\frac{1}{2}}_{\ell...\ell-c'+1-\mu_1..-\mu_{i-1}-\mu_i+1\ \mu_{i+1}..\mu_m}$$

$$= 0 \quad \text{as required.}$$

$S_{+1}\mathcal{J}_m = 0$ since we note to each monomomial of the form $\nabla^{\frac{1}{2}}_{..\mu_i=k..}\ \nabla^{-\frac{1}{2}}_{..-\mu_i=-k..}$ with $-k<\ell-c'-d'+1$ that is non-vanishing under S_{+1} there exists a term $\nabla^{\frac{1}{2}}_{..\mu_j=-k..}\ \nabla^{-\frac{1}{2}}_{..-\mu_j=k..}$ which together cancel under S_{+1}.

The raising operators W_{ab}, $b < a$, of $R_{2\ell+1}$ when applied to $\mathcal{F}_m$ give of course a null result.

It follows from (I-19) that

$$L_M = 2\sum_{i=\ell-c'+1}^{\ell} i + \sum_{i=\ell-c'-d'+1}^{\ell-c'} i = (2\ell+1-c')c' + \tfrac{1}{2}(2\ell+1-2c'-d')d'$$

Since each term in $\mathcal{F}_m$ has a coefficient of modulus one, the normalisation can be derived simply by counting the number of mononomials in $\mathcal{F}_m$. Hence

$$N = \sum_{\mu_1=1}^{M} \sum_{\mu_2=1}^{\mu_1} \cdots \sum_{\mu_m=1}^{\mu_{m-1}} 1$$

where M is the maximum number of different values that μ_1 (or μ_i) can take, i.e. $M = 2\ell+2-a-b-c'$. Now

$$\sum_{\mu_m=1}^{\mu_{m-1}} 1 = \mu_{m-1}$$

$$\sum_{\mu_{m-1}=1}^{\mu_{m-2}} \mu_{m-1} = \frac{1}{2!}\,\mu_{m-2}\,(\mu_{m-2}+1)$$

$$\sum_{\mu_{m-2}=1}^{\mu_{m-3}} \frac{1}{2!}\,\mu_{m-2}(\mu_{m-2}+1) = \frac{1}{3!}\,\mu_{m-3}(\mu_{m-3}+1)(\mu_{m-3}+2)$$

etc.

$$\text{So} \quad N = \frac{1}{m!} \prod_{r=0}^{m-1} (M+r) = \frac{(M+m-1)!}{m!(M-1)!}$$

Finally then $|\{2^{a}1^{b}\}[2^{c}1^{d}]L_{M}\rangle$

$$= \left[\frac{(a-c')!(2\ell+1-a-c'-b)!}{(2\ell+1-2c'-b)!}\right]^{\frac{1}{2}} \sum_{\mu_1>\mu_2>..>\mu_{a-c'}} (-1)^{\mu_1+\mu_2+..+\mu_{a-c'}}$$

$$\times \nabla^{\frac{1}{2}}_{\ell\ \ell-1..\ell-c'-d'+1\ \mu_1\mu_2..\mu_{a-c'}} \nabla^{-\frac{1}{2}}_{\ell\ \ell-1..\ell-c'+1-\mu_1-\mu_2..-\mu_{a-c'}} \tag{I-20}$$

To give a general formula for arbitrary L is a very much more difficult task. [0]S and $[1]\ell$ are special cases of $\mathcal{J}_m$; additionally formulas for [2]L and [11]L have been derived. Writing $|\{11\}[11]L\rangle$ as $N \sum_a \beta_a \nabla^{\frac{1}{2}}_{L-a\ a}$ and applying the L_{+1} condition, we get a set of simultaneous equations, namely

$$t^{1}_{L-\ell+1}\ \beta\nabla^{\frac{1}{2}}_{L-\ell\ \ell} + t^{1}_{\ell}\ \beta\nabla^{\frac{1}{2}}_{L-\ell+1\ \ell-1} = 0 \quad \text{(a)}$$

$$t^{1}_{L-\ell+2}\ \beta\nabla^{\frac{1}{2}}_{L-\ell+1\ \ell-1} + t^{1}_{\ell-1}\ \beta\nabla^{\frac{1}{2}}_{L-\ell+2\ \ell-2} = 0 \quad \text{(b)}$$

$$t^{1}_{\ell-1}\ \beta\nabla^{\frac{1}{2}}_{\ell-2\ L-\ell+2} + t^{1}_{L-\ell+2}\ \beta\nabla^{\frac{1}{2}}_{\ell-1\ L-\ell+1} = 0 \quad \text{(b)} \tag{I-21}$$

$$t^{1}_{\ell}\ \beta\nabla^{\frac{1}{2}}_{\ell-1\ L-\ell+1} + t^{1}_{L-\ell+1}\ \beta\nabla^{\frac{1}{2}}_{\ell L-\ell} = 0 \quad \text{(a)}$$

which has the solution

$$\beta_a = (-1)^a \prod_{y=a+1}^{\ell} \frac{t_{L-y+1}}{t_y} \qquad \text{(I-22)}$$

which is understood to be $(-1)^a = (-1)^{\ell}$ if $a = \ell$. Since the equations aa, bb ... etc. are equal the summation is restricted to $\frac{1}{2}(L+1) < a < \ell$, i.e.

$$|\{11\}[11]L\rangle = N \sum_{a=\frac{1}{2}(L+1)}^{\ell} \beta_a \, \nabla^{\frac{1}{2}}_{L-a} \, a$$

No solution exists if L is even as required by the branching rule. We get a similar solution for $|\{2\}[2]L\rangle$ namely

$$|\{2\}[2]L\rangle = N \sum_{a=L-\ell}^{\ell} \beta_a \, \nabla^{\frac{1}{2}}_{L-a} \, \nabla^{-\frac{1}{2}}_{a}$$

with the same β_a as for [11](22), the summation in this case being unrestricted. Note that

$$S_{+1}|\{2\}[2]L\rangle = N \sum_a (\beta_a \, \nabla^{\frac{1}{2}}_{L-a} \, a + \beta_{L-a} \, \nabla^{\frac{1}{2}}_{a} \, L-a)$$

so since $\beta_a = (-1)^L \beta_{L-a}$, this expression vanishes for L even, as required by the branching rule.

To find N we must evaluate the expression

$$\sum_a \beta_a^2 = \sum_a \prod_{y=a+1}^{\ell} \left(\frac{t^1_{L-y+1}}{t^1_y} \right)^2 \qquad \text{(I-23)}$$

with the appropriate limits for each case. We have that

$$\frac{t^1_a}{t^1_b} = \frac{(-1)^a \begin{pmatrix} \ell & 1 & \ell \\ -a & 1 & a-1 \end{pmatrix}}{(-1)^b \begin{pmatrix} \ell & 1 & \ell \\ -b & 1 & b-1 \end{pmatrix}} = \left[\frac{(\ell+a)(\ell-a+1)}{(\ell+b)(\ell-b+1)}\right]^{\frac{1}{2}}$$

so (I-23) becomes

$$\sum_a \prod_{y=a+1} \frac{(\ell+L-y+1)(\ell-L+y)}{(\ell+y)(\ell-y+1)} = \frac{(2\ell-L)!}{(2\ell)!L!} \sum_a \frac{(\ell+a)!(\ell+L-a)!}{(\ell-a)!(\ell-L+a)!}$$

$$= \frac{(2\ell-L)!L!}{(2\ell)!} \sum_a \binom{\ell+a}{\ell-L+a} \binom{\ell+L-a}{\ell-a}$$

$$= (\tfrac{1}{2})\frac{(2\ell-L)!L!}{(2\ell)!} \binom{2\ell+L+1}{2\ell-L} \qquad \text{(I-24)}$$

as a consequence of one of the many variants of the binomial addition formula. The $\frac{1}{2}$ occurs only in the restricted summation case of [11]. (I-24) implies that

$$N = \left[\frac{(2)(2\ell)!(2L+1)!}{L!(2\ell+1+L)!}\right]^{\frac{1}{2}}$$

so finally

$$|\{11\}[11]L\rangle = \left[\frac{2(2L+1)!(2\ell-L)!}{(L!)^2(2\ell+1+L)!}\right]^{\frac{1}{2}} \sum_{a=\frac{1}{2}(L+1)}^{\ell} (-1)^a$$

$$\left[\frac{(\ell+a)!(\ell+L-a)!}{(\ell-a)!(\ell-L+a)!}\right]^{\frac{1}{2}} \nabla^{\frac{1}{2}}_{L-a\ a} \qquad \text{(I-25a)}$$

and

$$|\{2\}[2]L\rangle = \left[\frac{(2L+1)!(2\ell-L)!}{(L!)^2(2\ell+1+L)!}\right]^{\frac{1}{2}} \sum_{a=L-\ell}^{\ell} (-1)^a$$

$$\left[\frac{(\ell+a)!(\ell+L-a)!}{(\ell-a)!(\ell-L+a)!}\right]^{\frac{1}{2}} \nabla^{\frac{1}{2}}_{L-a}\ \nabla^{-\frac{1}{2}}_{a} \qquad \text{(I-25b)}$$

To find the expansion of a three or more particle state of general L and greatest weight in SU_2, in lieu of a general formula, we must demand that

$$L_{+1} = \sum_b t^q_b\ X_{q\ b-q} \qquad \text{(I-2)}$$

and S_{+1} on the state be zero, giving a set of simultaneous equations, which in the general case will have a set of solutions corresponding to the multiplicity of L in the branching rule of $[2^c 1^d]$ upon restriction to R_3.

5. Semiconjugacy

In this section it is shown that once the states $|\{2^c1^d\}[2^c1^d]L\rangle$ have been calculated explicitly, all other general states may be written down. We start by noting that the branching rules given in Section 4 imply that a general state falls into two classes, namely

$$|\{2^{c+x}1^d\}[2^c1^d]L\rangle \quad \text{and} \quad |\{2^{c+x}1^{2\ell+1-2c-d}\}[2^c1^d]L\rangle.$$

We consider now the product state $|\{2^c1^d\}[2^c1^d]L\rangle|\{2^x\}[0]S\rangle$. Since the only unitary representation of the form $\{2^a1^b\}$ contained in the direct product $\{2^c1^d\} \times \{2^x\}$ is $\{2^{c+x}1^d\}$, the product state is proportional to $|\{2^{c+x}1^d\}[2^c1^d]L\rangle$, the first of two classes of a general state. Similarly $|\{2^c1^{2\ell+1-2c-d}\}[2^c1^d]L\rangle|\{2^x\}[0]S\rangle$ is proportional to $|\{2^{c+x}1^{2\ell+1-2c-d}\}[2^c1^d]L\rangle$, i.e. the second class. Since $|\{2^x\}[0]S\rangle$ is known (equals $\mathcal{F}_x$, Section 4) and $|\{2^c1^d\}[2^c1^d]L\rangle$ is assumed known, we now have the first class of a general state. To find the second class we have only to find how to form

$$|\{2^c1^{2\ell+1-2c-d}\}[2^c1^d]L\rangle \text{ given } |\{2^c1^d\}[2^c1^d]L\rangle.$$

For this, the operation of semiconjugacy is introduced and represented by $\mathcal{R}$. Associated with a given set $\mathcal{A}$ of m_ℓ quantum is a complementary set $\mathcal{Z}$, defined such that

$\mathcal{A} \cup \bar{\mathcal{A}} = \{\ell, \ell-1, \ldots 1, 0, -1, \ldots -\ell+1, -\ell\}$ and $\mathcal{A} \cap \bar{\mathcal{A}} = \varphi$ the null set, for example if $\ell = 2$ and $\mathcal{A} = \{2,1\}$ then $\bar{\mathcal{A}} = \{0,-1,-2\}$. Semiconjugacy is now defined by its action on a mononomial, namely

$$\nabla^{\frac{1}{2}}_{\mu_1 \ldots \mu_m} \nabla^{-\frac{1}{2}}_{\nu_1 \ldots \nu_n} = \bar{\nabla}^{\frac{1}{2}}_{\mu_1 \ldots \mu_m} \nabla^{-\frac{1}{2}}_{\nu_1 \ldots \nu_n} \qquad \text{(I-26)}$$

where

$$\bar{\nabla}^{\frac{1}{2}}_{\mu_1 \ldots \mu_m} = \nabla^{\frac{1}{2}}_{\mu'_1 \ldots \mu'_{2\ell+1-m}}$$

where $\{\mu'_1 \ldots \mu'_{2\ell+1-m}\}$ is the negative of the complementary set to $\{\mu_1 \ldots \mu_m\}$. For instance if $\mathcal{A} = \{2,1\}$ and $\ell = 2$, $\bar{\mathcal{A}} = \{0,-1,-2\}$ and the negative of this set is $\{210\}$. The phase given in the definition (I-26) of $\mathcal{R}$ (namely +1) holds only if $\mu_1 \ldots \mu_m$ and $\mu'_1 \ldots \mu'_{2\ell+1-m}$ are ordered after the fashion $\mu_1 > \mu_2 > \ldots > \mu_m$ and $\mu'_1 > \mu'_2 > \ldots > \mu'_{2\ell+1-m}$. The operation is equivalent to replacing spin up electrons only, with their corresponding holes, hence its name.

It remains to show that has the desired property that $\mathcal{R}|\{2^c 1^d\}[2^c 1^d]L\rangle = |\{2^c 1^{2\ell+1-2c-d}\}[2^c 1^d]L\rangle$, allowing the right hand state to be written down simply by placing a bar over the $\nabla^{\frac{1}{2}}$ of each mononomial in the expansion of the left hand state, assumed known. We see firstly that each mononomial $\bar{\nabla}^{\frac{1}{2}}_{q_1 \ldots q_{a+b}} \nabla^{-\frac{1}{2}}_{r_1 \ldots r_a}$ since if $q_1+q_2+\ldots+q_{a+b} = Q$ then the complementary set to q sums to -Q. Moreover

$$L_{+1}\nabla^{\frac{1}{2}}_{..\mu_i\ \mu_i-k..} = .. + (t^{1}_{\mu_i+1}\ \nabla^{\frac{1}{2}}_{..\mu_i+1\ \mu_i-k..}) + t^{1}_{\mu_1-k+1}\nabla^{\frac{1}{2}}_{..\mu_i\ \mu_i-k+1} + ..$$

where the first term does not exist if $\mu_{i-1} = \mu_i+1$ while

$$L_{+1}\overline{\nabla^{\frac{1}{2}}}_{...\mu_i\ \mu_i-k..} = L_{+1}\nabla^{\frac{1}{2}}_{(-\mu_i-1)-\mu_i+1\ -\mu_i+2..-\mu_i+k-1..}$$

$$= .. + (t^{1}_{-\mu_i}\nabla^{\frac{1}{2}}_{(-\mu_i)-\mu_i+1..-\mu_i+k-1..}) + t^{1}_{-\mu_i+k}\ \nabla^{\frac{1}{2}}_{(-\mu_i-1)\mu_i+1..\mu_i+k-2\ -\mu_i+k..} + ..$$

$$= .. + (t^{1}_{\mu_i+1}\ \overline{\nabla^{\frac{1}{2}}}_{..\mu_i+1\ \mu_i-k..}) + t_{\mu_i-k+1}\ \overline{\nabla^{\frac{1}{2}}}_{..\mu_i\mu_i-k+1} + ..$$

Hence the simultaneous equations derived by $\mathcal{R}$- transforming the L_{+1} simultaneous equations for the state $|\{2^{c_1}d\}[2^{c_1}d]>$ are again a set of simultaneous equations satisfying the L_{+1} condition.

We consider now the action of on the n-1 dimensional solution to the one pair submatrix of A (I-18)

$\sum_x(-1)^x\nabla^{\frac{1}{2}}_{q}\ x\ \nabla^{-\frac{1}{2}}_{r-x}$ where $q \equiv q_2q_2..q_{a+b-1}$ and $r \equiv r_1r_2..r_{a-1}$

$$\sum_x (-1)^x \nabla^{\frac{1}{2}}_q \times \nabla^{-\frac{1}{2}}_{r-x} = \sum_{x=-q_i} (-1)^{q_i} \nabla^{\frac{1}{2}}_{q-q_i} \nabla^{-\frac{1}{2}}_{r\ q_i} + (\nabla^{\frac{1}{2}}_{q\ 0} \nabla^{-\frac{1}{2}}_{r\ 0})$$

$$+ \sum_{\substack{x\neq 0 \\ \neq -q_i}} (-1)^x \nabla^{\frac{1}{2}}_q \times \nabla^{-\frac{1}{2}}_{r-x}$$

The zero term is bracketed, since if r_i or q_i equals zero it does not exist, so

$$\mathcal{R} \sum_x (-1)^x \nabla^{\frac{1}{2}}_q \times \nabla^{-\frac{1}{2}}_{r-x} = \sum_{q_i} (-1)^{q_i} M_{-q_i} \nabla^{\frac{1}{2}}_{q\dot{-}q_i} \nabla^{-\frac{1}{2}}_{r\ q_i} + (M_0 \nabla^{\frac{1}{2}}_{q\dot{-}0} \nabla^{-\frac{1}{2}}_{r\ 0})$$

$$+ \sum_{\substack{x\neq 0 \\ \neq -q_i}} (-1)^x M_x \nabla^{\frac{1}{2}}_{q\dot{-}x} \nabla^{-\frac{1}{2}}_{r\ x} \qquad \text{(I-27)}$$

where the first summation is through q_i, such that there exists a $q_j = -q_i$ in q, while M_g is the phase required to order $\nabla^{\frac{1}{2}}_{q\dot{-}g}$. So if g belongs to position k in $\nabla^{\frac{1}{2}}$ counting from the left, $M_g = (-1)^{k-a-b}$. $\bar{q}$ is taken as the negative of the complementary set to q, i.e.

$$\mathcal{R} \nabla^{\frac{1}{2}}_q = \bar{\nabla}^{\frac{1}{2}}_q = \nabla^{\frac{1}{2}}_{\bar{q}}$$

while $\dot{-}$ means "without", i.e. $\{2,1,0\} \dot{-} 0 = \{21\}$. The three summations of equation (I-27) above taken together are thus an instruction to take each q_i from $\bar{q}$ and place it in the spin down space. We wish now to find the position

i of -g in $\bar{q}$. To do so we reason that since the number of blanks in the sequence ℓ ℓ-1...g for the set of quantum numbers q + g is both equal to ℓ-g-k+1 and the position of -g in $\bar{q}$ counting from the <u>right</u>, then the position of -g equals the difference of the length of $\bar{q}$ and the <u>right</u> position of g plus one, i.e.

$$i = (2\ell+1)-a-b) - (\ell-g-k+1) + 1 = \ell+g+k+1-a-b$$

Finally then

$$\mathcal{R} \sum_x (-1)^x \nabla^{\frac{1}{2}}_{q} \times \nabla^{-\frac{1}{2}}_{r-x} = (-1)^{\ell+1} \sum_i (-1)^i \nabla^{\frac{1}{2}}_{q-q_i} \nabla^{-\frac{1}{2}}_{r\, g_i} \qquad \text{(I-28)}$$

This, however, is just proportional to the general type of equation we get if we demand that the states $\bar{\nabla}^{\frac{1}{2}}_{q_1..q_{a+b}} \nabla^{-\frac{1}{2}}_{r_1..r_a}$ satisfy the S_{+1} condition (c.f. (I-4)). Conversely, we find that any S_{+1} equation for the $\nabla^{\frac{1}{2}}_{q_1..q_{a+b}} \nabla^{-\frac{1}{2}}_{r_1..r_a}$ states transform under to a single pair $R_{2\ell+1}$ condition (I-24) for $\bar{\nabla}^{\frac{1}{2}}_{q_1..q_{a+b}} \nabla^{-\frac{1}{2}}_{r_1..r_a}$. Since can clearly be applied in the reverse sense (i.e. from $\bar{\nabla}$ to ∇) giving the same result we have that the <u>total</u> set of equations required to solve for the state $|\{2^c1^d\}[2^c1^d]L\rangle$ is identical apart from a barred $\nabla^{\frac{1}{2}}$ to the <u>total</u> set of equations for $|\{2^c1^d\}[2^c1^d]L\rangle$. Since $\bar{\nabla}^{\frac{1}{2}}_{q_1..q_{a+b}} \nabla^{-\frac{1}{2}}_{r_1..r_a}$ has 2ℓ-1-a-b terms in the spin up space and M_S and M_L are maximum, we have as required

$$\mathcal{R}\,|\{2^{c}1^{d}\}[2^{c}1^{d}]L\rangle \;=\; |\{2^{c}1^{2\ell+1-2c-d}\}[2^{c}1^{d}]L\rangle \qquad \text{(I-29)}$$

Now since a general state is proportional to the product of $\{2^{c}1^{d}\}[2^{c}1^{d}]L\rangle$ or $|\{2^{c}1^{d}\}[2^{c}1^{d}]L\rangle$ with $|\{2^{x}\}[0]S\rangle$ it is clear that the proportionality constant is dependent only on the values of c and d and is thus equal to the normalisation of $\mathcal{G}_{x}$ divided by the normalisation of $|\{2^{x}\}[0]S\rangle$, i.e. is equal to

$$\left[\frac{(2\ell+1-2c-d-x)!(2\ell+1)!}{(2\ell+1-2c-d)!(2\ell+1-x)!}\right]^{\frac{1}{2}}$$

6. The d-Shell

It has been shown how to reduce the problem of constructing atomic wavefunctions in the $U_{2\ell+1} \supset R_{2\ell+1} \supset R_{3}$ to finding only the states $|\{2^{c}1^{d}\}[2^{c}1^{d}]L\rangle$. Unfortunately, it has not been possible to find a closed algebraic expression for these terms in general (with the exception of a few special cases given in Section 4) so they must be found by solving the set of simultaneous equations given by the L_{+1} and S_{+1} conditions, and applying additionally the single paired condition (I-18) given in Section 3. Even this may not be enough; since in Section 3 only one solution, corresponding to one eigenvalue, could be given to the multipaired case (I-19) it may happen that some of the eigenvalues for two or more pairs are also equal to the p

value (I-8) of the state in question. Any attempt to solve for this state with only zero and one pair, will give a vanishing result. In practise this serves as a guide to finding which states are of this type.

In the d shell the only term of this type is $|\{22\}[22]S\rangle$. The double paired submatrix for this case has eigenvalues 10, 5 (four times) and 2 (five times). The eigenvalue of 10 being the same as the p value for $|\{22\}[0]S\rangle$ corresponds to the doubly paired solution to this state, namely $\mathcal{J}_2$. The eigenvalue of 2 equals the p value for $|\{22\}[22]S\rangle$ and gives an eigenstate spanning a five dimensional space, described by the following equations

$$\alpha \nabla^{\frac{1}{2}}_{2\ 1}\nabla^{-\frac{1}{2}}_{-1-2} - \alpha \nabla^{\frac{1}{2}}_{0-1}\nabla^{-\frac{1}{2}}_{1\ 0} + \alpha \nabla^{\frac{1}{2}}_{0-2}\nabla^{-\frac{1}{2}}_{2\ 0} - \alpha \nabla^{\frac{1}{2}}_{-1-2}\nabla^{-\frac{1}{2}}_{2\ 1} = 0$$

$$\alpha \nabla^{\frac{1}{2}}_{2\ 0}\nabla^{-\frac{1}{2}}_{0-2} - \alpha \nabla^{\frac{1}{2}}_{1-1}\nabla^{-\frac{1}{2}}_{1-1} + \alpha \nabla^{\frac{1}{2}}_{1-2}\nabla^{-\frac{1}{2}}_{2-1} + \alpha \nabla^{\frac{1}{2}}_{1-2}\nabla^{-\frac{1}{2}}_{2\ 1} = 0$$

$$\alpha \nabla^{\frac{1}{2}}_{2-1}\nabla^{-\frac{1}{2}}_{1-2} - \alpha \nabla^{\frac{1}{2}}_{1-1}\nabla^{-\frac{1}{2}}_{1-1} + \alpha \nabla^{\frac{1}{2}}_{0-2}\nabla^{-\frac{1}{2}}_{2\ 0} - \alpha \nabla^{\frac{1}{2}}_{-1-2}\nabla^{-\frac{1}{2}}_{2\ 1} = 0$$

$$\alpha_{\nabla_1^{\frac{1}{2}}{}_0\nabla_0^{-\frac{1}{2}}{}_{-1}} \quad -\alpha_{\nabla_1^{\frac{1}{2}}{}_{-1}\nabla_1^{-\frac{1}{2}}{}_{-1}} \quad -\alpha_{\nabla_1^{\frac{1}{2}}{}_{-2}\nabla_2^{-\frac{1}{2}}{}_{-1}} \quad +\alpha_{\nabla_0^{\frac{1}{2}}{}_{-1}\nabla_1^{-\frac{1}{2}}{}_0}$$

$$-\alpha_{\nabla_0^{\frac{1}{2}}{}_{-2}\nabla_2^{-\frac{1}{2}}{}_0} \quad +\alpha_{\nabla_{-1}^{\frac{1}{2}}{}_{-2}\nabla_2^{-\frac{1}{2}}{}_1} = 0$$

This taken with the L_{+1} and S_{+1} equations gives the expansion of $|\{22\}[22]S\rangle$ as tabulated in Table I. There is no single paired condition for this state, for if it has one pair it has two.

As an example the equations for the state $|\{21\}[21]D\rangle$ are displayed. $R_{2\ell+1}$ equation

$$\alpha_{\nabla_2^{\frac{1}{2}}{}_1\nabla_{-1}^{-\frac{1}{2}}} \quad -\alpha_{\nabla_2^{\frac{1}{2}}{}_0\nabla_0^{-\frac{1}{2}}} \quad +\alpha_{\nabla_{2-1}^{\frac{1}{2}}\nabla_1^{-\frac{1}{2}}} \quad -\alpha_{\nabla_{2-2}^{\frac{1}{2}}\nabla_2^{-\frac{1}{2}}} = 0$$

L_{+1} equations

$$t_1^1\alpha_{\nabla_2^{\frac{1}{2}}{}_0\nabla_0^{-\frac{1}{2}}} + t_0^1\alpha_{\nabla_2^{\frac{1}{2}}{}_1\nabla_{-1}^{-\frac{1}{2}}} = 0$$

$$t_2^1\alpha_{\nabla_1^{\frac{1}{2}}{}_0\nabla_1^{-\frac{1}{2}}} + t_0^1\alpha_{\nabla_{2-1}^{\frac{1}{2}}\nabla_1^{-\frac{1}{2}}} + t_1^1\alpha_{\nabla_2^{\frac{1}{2}}{}_0\nabla_0^{-\frac{1}{2}}} = 0$$

$$t_2^1\alpha_{\nabla_{1-1}^{\frac{1}{2}}\nabla_2^{-\frac{1}{2}}} + t_{-1}^1\alpha_{\nabla_{2-2}^{\frac{1}{2}}\nabla_2^{-\frac{1}{2}}} + t_2^1\alpha_{\nabla_{2-1}^{\frac{1}{2}}\nabla_1^{-\frac{1}{2}}} = 0$$

S_{+1} equation

$$\alpha\, {}^{\frac{1}{2}}\nabla^{\frac{1}{2}}_{2}\ {}^{-\frac{1}{2}}\nabla_{-1}^{-\frac{1}{2}} - \alpha\, {}^{\frac{1}{2}}\nabla^{\frac{1}{2}}_{2-1}\nabla_{1}^{-\frac{1}{2}} + \alpha\, {}^{\frac{1}{2}}\nabla^{\frac{1}{2}}_{1-1}\nabla_{2}^{-\frac{1}{2}} = 0$$

Since $\frac{t^{1}_{1}}{t^{1}_{2}} = \sqrt{\frac{3}{2}}$ the normalised solution to these equations is

$$\sqrt{\frac{3}{28}}\,({}^{\frac{1}{2}}\nabla^{\frac{1}{2}}_{2}\ {}^{-\frac{1}{2}}\nabla_{-1}^{-\frac{1}{2}} - {}^{\frac{1}{2}}\nabla^{\frac{1}{2}}_{2}\ {}^{-\frac{1}{2}}\nabla_{0}^{-\frac{1}{2}} - \tfrac{1}{3}\,{}^{\frac{1}{2}}\nabla^{\frac{1}{2}}_{2-1}\nabla_{1}^{-\frac{1}{2}} + \tfrac{5}{3}\,{}^{\frac{1}{2}}\nabla^{\frac{1}{2}}_{2-2}\nabla_{2}^{-\frac{1}{2}}$$

$$- \tfrac{4}{3}\,{}^{\frac{1}{2}}\nabla^{\frac{1}{2}}_{1-1}\nabla_{2}^{-\frac{1}{2}} + \tfrac{8}{3}\,{}^{\frac{1}{2}}\nabla^{\frac{1}{2}}_{1}\ {}^{-\frac{1}{2}}\nabla_{1}^{-\frac{1}{2}})$$

One point to note; for the $|\{22\}[22]L\rangle$ states the S_{+1} condition becomes

$$\alpha\, {}^{\frac{1}{2}}\nabla^{\frac{1}{2}}_{a}\ {}^{b}\nabla_{c}^{-\frac{1}{2}}\ {}^{a} - \alpha\, {}^{\frac{1}{2}}\nabla^{\frac{1}{2}}_{a}\ {}^{c}\nabla_{b}^{-\frac{1}{2}}\ {}^{d} = 0$$

i.e.

$$\alpha\, {}^{\frac{1}{2}}\nabla^{\frac{1}{2}}_{a}\ {}^{b}\nabla_{c}^{-\frac{1}{2}}\ {}^{a} \qquad \alpha\, {}^{\frac{1}{2}}\nabla^{\frac{1}{2}}_{c}\ {}^{a}\nabla_{a}^{-\frac{1}{2}}\ {}^{b}$$

which allows us, with the exception of L = 0 (it has other S_{+1} equations as well), to nearly half the number of unknowns.

The states of the form $|\{2^{c}1^{d}\}[2^{c}1^{d}]L\rangle$ are found tabulated in Table I.

7. Conclusions

In this Chapter the atomic states $|\{2^a 1^b\}[2^c 1^d]L\rangle$ for maximum M_L and M_S and for $2a+b \leq 2\ell+1$ have been constructed in the scheme $U_{2\ell+1} \supset R_{2\ell+1} \supset R_3$. Clearly states with $2a+b > 2\ell+1$ can be derived by using particle hole equivalence[1,5]; in terms of my notation, one would simply place a bar over both $\nabla^{\frac{1}{2}}$ and $\nabla^{-\frac{1}{2}}$ to derive the hole state equivalent to a given particle state. The form of the states I use imply a phase convention, for the state $\nabla^{\frac{1}{2}}_{3\ 2\ 1}\ \nabla^{-\frac{1}{2}}_{-2-1}$ could equally well be written as $\nabla^{\frac{1}{2}}_{3\ 2\ 1}\ \nabla^{-\frac{1}{2}}_{-1-2}$ (any other permutation of m_ℓ indices is clearly equivalent to one of these two states). In general then one cannot expect the phase of any cfp's derived using this basis to agree with that of Racah[1], or Nielson and Koster[25] unless one deliberately defined the phase of the states to do so. However, one is guaranteed a self-consistent set of phases that is all that is required practically. Defining semiconjugacy makes it necessary to calculate only the states $\{2^c 1^d\}[2^c 1^d]L\rangle$; for these states however, no general closed algebraic expression could be found, in fact in view of the immense combinatorial complexity of this problem, it seems doubtful that such an expression exists.

TABLE I

The States $|\{2^c 1^d\}[2^c 1^d]L\rangle$ of the d Shell

State Quantum Numbers	Mononomial expansion
$\{0\}[0]S$	-
$\{1\}[1]D$	$v^{\frac{1}{2}}_{2}$
$\{11\}[11]F$	$v^{\frac{1}{2}}_{2\ 1}$
$\{11\}[11]P$	$\frac{1}{\sqrt{5}}(\sqrt{2}v^{\frac{1}{2}}_{-1\ 2} - \sqrt{3}v^{\frac{1}{2}}_{0\ 1})$
$\{2\}[2]G$	$v^{\frac{1}{2}}_{2}\ v^{-\frac{1}{2}}_{2}$
$\{2\}[2]D$	$\frac{1}{\sqrt{7}}(\sqrt{2}v^{\frac{1}{2}}_{0}v^{-\frac{1}{2}}_{2} - \sqrt{3}v^{\frac{1}{2}}_{1}v^{-\frac{1}{2}}_{1} + \sqrt{2}v^{\frac{1}{2}}_{2}v^{-\frac{1}{2}}_{0})$
$\{21\}[21]H$	$v^{\frac{1}{2}}_{2\ 1}\ v^{-\frac{1}{2}}_{2}$
$\{21\}[21]G$	$\frac{1}{\sqrt{5}}\ (\sqrt{3}v^{\frac{1}{2}}_{2\ 1}\ v^{-\frac{1}{2}}_{1} - \sqrt{2}\ v^{\frac{1}{2}}_{2\ 0}\ v^{-\frac{1}{2}}_{2})$
$\{21\}[21]F$	$\frac{1}{\sqrt{12}}\ (v^{\frac{1}{2}}_{2\ 1}v^{-\frac{1}{2}}_{0} - v^{\frac{1}{2}}_{2\ 0}v^{-\frac{1}{2}}_{1} + \sqrt{6}v^{\frac{1}{2}}_{2-1}v^{-\frac{1}{2}}_{2} - 2v^{\frac{1}{2}}_{1\ 0}v^{-}$
$\{21\}[21]D$	$\sqrt{\frac{3}{28}}\ (v^{\frac{1}{2}}_{2\ 1}v^{-\frac{1}{2}}_{-1} - v^{\frac{1}{2}}_{2\ 0}v^{-\frac{1}{2}}_{0} - \frac{1}{3}v^{\frac{1}{2}}_{2-1}v^{-\frac{1}{2}}_{1} + \frac{5}{3}v^{\frac{1}{2}}_{2-2}v^{-\frac{1}{2}}_{2}$ $- \frac{4}{3}v^{\frac{1}{2}}_{1-1}v^{-\frac{1}{2}}_{2} + \sqrt{\frac{8}{3}}v^{\frac{1}{2}}_{1\ 0}v^{-\frac{1}{2}}_{1})$
$\{21\}[21]P$	$\sqrt{\frac{8}{35}}\ (\frac{3}{4}v^{\frac{1}{2}}_{1\ 0}v^{-\frac{1}{2}}_{0} - v^{\frac{1}{2}}_{1\ 2}v^{-\frac{1}{2}}_{-2} - \frac{3}{4}v^{\frac{1}{2}}_{1-1}v^{-\frac{1}{2}}_{1} - \frac{1}{2}v^{\frac{1}{2}}_{1-2}v^{-\frac{1}{2}}_{2}$ $+ \frac{1}{2\sqrt{6}}v^{\frac{1}{2}}_{2-1}v^{-\frac{1}{2}}_{0} - \sqrt{\frac{2}{3}}v^{\frac{1}{2}}_{2\ 0}v^{-\frac{1}{2}}_{-1} + \frac{5}{2\sqrt{6}}v^{\frac{1}{2}}_{0-1}v^{-\frac{1}{2}}_{2}$ $+ \frac{1}{2}v^{\frac{1}{2}}_{2-2}v^{-\frac{1}{2}}_{1})$

Table I (contd)

$\{22\}[22]I \qquad \nabla^{\frac{1}{2}}_{2\ 1}\nabla^{-\frac{1}{2}}_{2\ 1}$

$\{22\}[22]G \qquad \sqrt{\frac{1}{33}}\,(\nabla^{\frac{1}{2}}_{2\ 1}\nabla^{-\frac{1}{2}}_{2-1} + 2\nabla^{\frac{1}{2}}_{2\ 0}\nabla^{-\frac{1}{2}}_{2\ 0} + \nabla^{\frac{1}{2}}_{2-1}\nabla^{-\frac{1}{2}}_{2\ 1}$

$- 3\sqrt{\tfrac{3}{2}}\,\nabla^{\frac{1}{2}}_{2\ 1}\nabla^{-\frac{1}{2}}_{1\ 0} - 3\sqrt{\tfrac{3}{2}}\,\nabla^{\frac{1}{2}}_{1\ 0}\nabla^{-\frac{1}{2}}_{2\ 1}$

$\{22\}[22]F \qquad \sqrt{\frac{3}{40}}\,(\nabla^{\frac{1}{2}}_{2\ 1}\nabla^{-\frac{1}{2}}_{1-1} - \nabla^{\frac{1}{2}}_{2\ 0}\nabla^{-\frac{1}{2}}_{1\ 0} + 2\nabla^{\frac{1}{2}}_{2-2}\nabla^{-\frac{1}{2}}_{1\ 2} + \nabla^{\frac{1}{2}}_{1-1}\nabla^{-\frac{1}{2}}_{2-1}$

$- \nabla^{\frac{1}{2}}_{1\ 0}\nabla^{-\frac{1}{2}}_{2\ 0} + 2\nabla^{\frac{1}{2}}_{2\ 1}\nabla^{-\frac{1}{2}}_{2-2} - \sqrt{\tfrac{2}{3}}\nabla^{\frac{1}{2}}_{2\ 0}\nabla^{-\frac{1}{2}}_{2-1} - \sqrt{\tfrac{2}{3}}\nabla^{\frac{1}{2}}_{2-1}\nabla^{-\frac{1}{2}}_{2\ 0}$

$\{22\}[22]D \qquad \sqrt{\frac{1}{21}}\,(\nabla^{\frac{1}{2}}_{2-1}\nabla^{-\frac{1}{2}}_{1\ 0} + \nabla^{\frac{1}{2}}_{2\ 0}\nabla^{-\frac{1}{2}}_{2-2} - \sqrt{\tfrac{3}{2}}\nabla^{\frac{1}{2}}_{2\ 1}\nabla^{-\frac{1}{2}}_{1-2}$

$-\sqrt{6}\nabla^{\frac{1}{2}}_{1\ 0}\nabla^{-\frac{1}{2}}_{1\ 0} + \nabla^{\frac{1}{2}}_{1\ 0}\nabla^{-\frac{1}{2}}_{2-1} + \nabla^{\frac{1}{2}}_{2-2}\nabla^{-\frac{1}{2}}_{2\ 0} - \sqrt{\tfrac{3}{2}}\nabla^{\frac{1}{2}}_{1-2}\nabla^{-\frac{1}{2}}_{2\ 1}$

$+ \nabla^{\frac{1}{2}}_{2\ 0}\nabla^{-\frac{1}{2}}_{1-1} - \sqrt{6}\,\nabla^{\frac{1}{2}}_{2-1}\nabla^{-\frac{1}{2}}_{2-1} + \nabla^{\frac{1}{2}}_{1-1}\nabla^{-\frac{1}{2}}_{2\ 0})$

$\{22\}[22]S \qquad \sqrt{\frac{3}{70}}\,(\nabla^{\frac{1}{2}}_{2\ 1}\nabla^{-\frac{1}{2}}_{-1-2} - \nabla^{\frac{1}{2}}_{0-1}\nabla^{-\frac{1}{2}}_{1\ 0} - \nabla^{\frac{1}{2}}_{0-2}\nabla^{-\frac{1}{2}}_{2\ 0} - \tfrac{1}{3}\nabla^{\frac{1}{2}}_{1-2}\nabla^{-\frac{1}{2}}_{2-1}$

$+ \tfrac{4}{3}\nabla^{\frac{1}{2}}_{1-1}\nabla^{-\frac{1}{2}}_{2-2} + \sqrt{\tfrac{8}{3}}\nabla^{\frac{1}{2}}_{1\ 0}\nabla^{-\frac{1}{2}}_{1-2} + 2\sqrt{\tfrac{2}{3}}\nabla^{\frac{1}{2}}_{2-1}\nabla^{-\frac{1}{2}}_{0-1}$

$+$ their opposites*

$+ (\tfrac{5}{3}\nabla^{\frac{1}{2}}_{2-2}\nabla^{-\frac{1}{2}}_{2-2} - \tfrac{1}{3}\nabla^{\frac{1}{2}}_{1-1}\nabla^{-\frac{1}{2}}_{1-1})\ )$

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* e.g. the opposite of $-\tfrac{1}{3}\nabla^{\frac{1}{2}}_{1-2}\nabla^{-\frac{1}{2}}_{2-1}$ is $-\tfrac{1}{3}\nabla^{\frac{1}{2}}_{2-1}\nabla^{-\frac{1}{2}}_{1-2}$.

C H A P T E R I I

A REFINEMENT OF REDMOND'S FORMULA APPLIED TO d-SHELL COEFFICIENTS OF FRACTIONAL PARENTAGE

1. Introduction

in 1954 Redmond[26] derived his formula giving an iterative relation for one body coefficients of fractional parentage (cfp's) for equivalent fermions. Simplified rederivations have been given by many authors[27-29] and the original formula has been generalized to cover n-body cfp's connecting states of general permutational symmetry[27,29]. However, the use of Redmond's (generalized) formula as a practical technique for calculating cfp's is cumbersome, except under very special circumstances[29,30], for several reasons: The Redmond states are non-orthogonal and essentially un-normalized, in that extra steps are required to evaluate normalization constants. Moreover, as has been shown by Nutter and Nielson[31], elaborate projection procedures must be followed in order to derive from Redmond cfp's, cfp's connected states whose auxiliary quantum numbers are fixed from other considerations (in particular whose auxiliary quantum numbers are chosen such that the state transforms according to representations of certain continuous groups, as is the case in Racah's[1] state classification scheme). In this report these disadvantages are overcome

by showing how to expand the Redmond cfp in terms of cfp's of states with arbitrary auxiliary quantum numbers (Section 2).

The method is then applied to derive formulae as opposed to simply numerical values for the squares of atomic d shell one body cfp's (Section 3) with the auxiliary quantum numbers given by the representations of the group R_5. Numerical values for these cfp's have long been known[22,25,27], but attempts to give formulae have met with only limited success, due to the complexity of the R_5 generator matrix elements in the basis specified by the non-canonical $R_5 \supset R_3$ group chain[32]. In Section 4 a short discussion on two body cfp's is given. Numerical values for these have been given by Jucys et al[33].

2. The Expansion of the Redmond State

In this section the generalization of Redmond's formula for n-body cfp's of antisymmetric states is derived by the method of Horie[28]. The resulting Redmond cfp is then expanded in terms of cfp's of arbitrarily defined orthonormal states.

Horie defines an antisymmetrizer

$$\mathcal{A}^{(n)} = \frac{1}{n!} \sum_p (-1)^p P$$

where the summation is through all n! permutations P of the symmetric group S_n and $(-1)^p$ is the parity of the permutation. $\mathcal{A}^{(n)}$ acts on an arbitrary n particle state $|\alpha JM\rangle$ (here α is an auxiliary quantum number, J is the angular momentum of the state and M its z projection) and antisymmetrizes it. Thus

$$|(\alpha)JM\rangle = N_{\alpha J}\mathcal{A}^{(n)}|\alpha JM\rangle$$

where $N_{\alpha J}$ is a normalization constant and the brackets around α mean that the state is antisymmetrized.

If the wavefunction $|\alpha'J',\alpha"J";JM\rangle$ is defined as

$$|\alpha'J',\alpha"J";JM\rangle = \sum_{M,M'} |\alpha'J'M'\rangle_{n-m}|\alpha"J"M"\rangle_m\langle J'M'J"M"|JM\rangle \tag{II-1}$$

where the subscript to $|\alpha JM\rangle$ specifies the number of particles associated with that state, then

$$|(\alpha_1J_1,\alpha_2J_2);JM\rangle = N(\alpha_1J_1,\alpha_2J_2;J)\mathcal{A}^{(n)}|\alpha_1J_1,\alpha_2J_2;JM\rangle \tag{II-2}$$

However, by the definition of cfp's we have

$$|(\alpha)JM\rangle = \sum_{\alpha'J',\alpha"J"} |\alpha'J',\alpha"J";JM\rangle\langle\alpha'J',\alpha"J"|\}(\alpha)J\rangle \tag{II-3}$$

so assuming that the states $|\alpha'J'M'\rangle_{n-m}$ and $|\alpha"J"M"\rangle_m$ are orthonormal it follows that

$$\langle\alpha'J',\alpha"J"|\}(\alpha)J\rangle = \langle\alpha'J',\alpha"J";JM|(\alpha)JM\rangle \tag{II-4}$$

From (II-2) and (II-4) therefore

$$\frac{\langle \alpha' J', \alpha'' J'' | \} (\alpha_1 J_1, \alpha_2 J_2); J \rangle}{N(\alpha_1 J_1, \alpha_2 J_2; J)} = \langle \alpha' J', \alpha'' J''; JM | \mathcal{A}^{(n)} | \alpha_1 J_1, \alpha_2 J_2; JM \rangle \qquad \text{(II-5)}$$

Horie now expands $\mathcal{A}^{(n)}$ in terms of antisymmetrizers for n_1 and n_2 particles ($n_1+n_2 = n$) to obtain the generalized Redmond's formula, viz.

$$\langle \alpha' J', \alpha'' J''; JM | \mathcal{A}^{(n)} | \alpha_1 J_1, \alpha_2 J_2; JM \rangle$$

$$= \sum_p (-1)^{p(n_2-m+p)} \binom{m}{p} \binom{n-m}{n_1-p} \Big/ \binom{n}{n_1} \Sigma \langle (\alpha') J' \{ | \alpha_1' J_1', \alpha_2' J_2' \rangle$$

$$\times \langle (\alpha'') J'' \{ | \alpha_1'' J_1'', \alpha_2'' J_2'' \rangle \langle J_1' J_2' (J') J_1'' J_2'' (J''); J | J_1' J_1'' (J_1) J_2' J_2'' (J_2); J \rangle$$

$$\times \langle \alpha_1' J_1', \alpha_1'' J_1'' | \} (\alpha_1) J_1 \rangle \langle \alpha_2' J_2', \alpha_2'' J_2'' | \} (\alpha_2) J_2 \rangle \qquad \text{(II-6)}$$

where the second summation is through the states $\alpha_1' J_1'$, $\alpha_2' J_2'$, $\alpha_1'' J_1''$ and $\alpha_2'' J_2''$ containing n_1-p, n_2-m+p, p and m-p particles, respectively. The bracket in the middle of the formula is a transformation coefficient between the coupling schemes of four angular momenta, and is proportional to a 9j symbol. The Redmond cfp is thus given in terms of cfp's coupling to less than n particles, via (II-5) and (II-6). The normalization constant $N(\alpha_1 J_1, \alpha_2 J_2; J)$ is calculated by noting that since $\mathcal{A}^{(n)}$ is hermitian

$$\frac{1}{N^2_{\alpha J}} = \langle \alpha JM | \mathcal{A}^{(n)} | \alpha JM \rangle \qquad \text{(II-7)}$$

so $N(\alpha_1 J_1, \alpha_2 J_2; J)$ is found by deriving the matrix element $\langle \alpha_1 J_1, \alpha_2 J_2; JM | \mathcal{A}^{(n)} | \alpha_1 J_1, \alpha_2 J_2; JM \rangle$ from (II-6).

To expand the Redmond cfp's in terms of the cfp's of the arbitrarily defined orthonormal states $|(\alpha)JM\rangle$ one looks more closely at the action of $\mathcal{A}^{(n)}$ on the state $|\alpha_1 J_1, \alpha_2 J_2; JM\rangle$. We have

$$\mathcal{A}^{(n)} |\alpha_1 J_1, \alpha_2 J_2; JM\rangle = \sum_{(\alpha)} |(\alpha)JM\rangle\langle(\alpha)JM| \mathcal{A}^{(n)} |\alpha_1 J_1, \alpha_2 J_2; JM\rangle$$

$$= \sum_{(\alpha)} |(\alpha)JM\rangle\langle(\alpha)JM|\alpha_1 J_1, \alpha_2 J_2; JM\rangle$$

since $\mathcal{A}^{(n)}$ is hermitian

$$\equiv \sum_{(\alpha)} |(\alpha)\ JM\rangle\langle(\alpha)J|\}\alpha_1 J_1, \alpha_2 J_2; J\rangle$$

by (II-4)

$$\langle \alpha' J' M', \alpha'' J'' M''; JM | \mathcal{A}^{(n)} | \alpha_1 J_1 M_1, \alpha_2 J_2 M_2; JM \rangle$$

$$= \sum_{(\alpha)} \langle (\alpha) J \{ | \alpha_2 J_2, \alpha_1 J_1 \rangle \langle \alpha' J', \alpha'' J'' | \} (\alpha) J \rangle \qquad \text{(II-8)}$$

This then taken with (II-6) gives an iterative relation between cfp's of the states $|(\alpha)JM\rangle$.

viz. $$\sum_{(\alpha)} \langle(\alpha)J\{|\alpha_2 J_2, \alpha_1 J_1\rangle\langle\alpha' J', \alpha'' J''|\}(\alpha)J\rangle$$

$$= \sum_p (-1)^{p(n_2-m+p)} \binom{m}{p} \binom{n-m}{n_1-p} \Big/ \binom{n}{n_1} \Sigma \langle(\alpha')J'\{|\alpha_1' J_1', \alpha_2 J_2'\rangle$$

$$\times \langle(\alpha'')J''\{|\alpha_1'' J_1'', \alpha_2'' J_2''\rangle\langle J_1' J_2'(J')J_1'' J_2''(J''); J|J_1' J_1''(J_1) J_2' J_2''(J_2); J\rangle$$

$$\times \langle\alpha_1' J_1', \alpha_1'' J_1''|\}(\alpha_1)J_1\rangle\langle\alpha_2' J_2', \alpha_2'' J_2''|\}(\alpha_2)J_2\rangle \qquad \text{(II-9)}$$

Innes[29] has noted the special case of one body cfp's of equivalent electron states classified by the seniority scheme[5].

3. d-Shell One Body cfp's

In this section, formula (II-9) is applied to atomic states of the d shell, specified (completely) according to the representations of the groups $(U_5 \supset R_5 \supset R_3) \times SU_2$, i.e. the state will be written as $|d^n[2^a 1^b]LS\rangle$ where n is the particle number, $[2^a 1^b]$ is an R_5 representation greatest weight label, and S and L are the spin (SU_2) and orbital (R_3) quantum numbers respectively (n and S taken together specify the U_5 representation, so this is suppressed).

For this case (II-9) becomes

$$\sum_{\alpha} \langle d^{n-1}\alpha_1 L_1 S_1 + d|\}d^n \alpha LS\rangle\langle d^{n-1}\alpha' L'S' + d|\}d^n \alpha LS\rangle$$

$$= \frac{1}{n}\left[\delta(\psi_1,\psi') + (n-1)\sum_{\psi_1'}\langle d^{n-2}\alpha_1' L_1' S_1' + d|\}d^{n-1}\alpha_1 L_1 S_1\rangle\right.$$

$$\times \langle d^{n-2}\alpha_1' L_1' S_1' + d|\}d^{n-1}\alpha' L'S'\rangle(-1)^t\{[S_1][L_1][S'][L']\}^{\frac{1}{2}}$$

$$\times \begin{Bmatrix} S_1 & \frac{1}{2} & S_1' \\ S' & \frac{1}{2} & S \end{Bmatrix} \begin{Bmatrix} L_1 & 2 & L_1' \\ L' & 2 & L \end{Bmatrix} \qquad \text{(II-10)}$$

where $t = S_1 + S' + L_1 + L'$, $[x] = 2x+1$ and ψ is the set of quantum numbers αLS.

To evaluate one-body cfp's we note firstly that for $R_{2\ell+1}$

$$[2^a 1^b]\times[1] = [32^{a-1}1^b] + [2^{a+1}1^{b-1}] + [2^a 1^{b+1}] + [2^{a-1}1^{b+1}] + [2^a 1^{b-1}] \qquad \text{(II-11)}$$

before modification rules are applied[23,24], provided that the exponents on the right hand side are non-negative (otherwise the term vanishes). This formula can be easily derived using Littlewood's methods[7,23]. In electron states states characterized by $[32^{a-1}1^b]$ never occur. However, if S is the spin associated with the parent state $[2^a 1^b]$, then the daughter state can have spin either $S+\frac{1}{2}$ or $S-\frac{1}{2}$, which in turn (through the $U_5 \supset R_5$ branching rules) can only be associated with the representations $[2^a 1^{b+1}]$

and $[2^{a-1}1^{b+1}]$ $(S+\frac{1}{2})$ or $[2^{a+1}1^{b-1}]$ or $[2^{a}1^{b-1}]$ $(S-\frac{1}{2})$.
Hence if in (II-10) we put $\alpha_1 = \alpha'$, $S_1 = S'$, $L_1 = L'$ the left hand side becomes

$$\langle d^{n-1}[2^{a}1^{b}]L_1S_1+d|\}d^{n}[2^{a}1^{b+1}]LS_1+\tfrac{1}{2}\rangle^2$$

$$+ \langle d^{n-1}[2^{a}1^{b}]L_1S_1+d|\}d^{n}[2^{a-1}1^{b+1}]LS_1+\tfrac{1}{2}\rangle^2 \qquad \text{(II-12a)}$$

or

$$\langle d^{n-1}[2^{a}1^{b}]L_1S_1+d|\}d^{n}[2^{a+1}1^{b-1}]LS_1-\tfrac{1}{2}\rangle^2$$

$$+ \langle d^{n-1}[2^{a}1^{b}]L_1S_1+d|\}d^{n}[2^{a}1^{b-1}]LS_1-\tfrac{1}{2}\rangle^2 \qquad \text{(II-12b)}$$

In building up the cfp's the second terms of (II-12) can be given in terms of cfp's already known through Racah factorization and reciprocity[1].

e.g.

$$\langle d^{n-1}[2^{a}1^{b}]L_1S_1+d|\}d^{n}[2^{a}1^{b-1}]LS_1-\tfrac{1}{2}\rangle^2$$

$$= \langle d^{n-1}[2^{a}1^{b}]S_1|\}d^{n}[2^{a}1^{b-1}]S_1-\tfrac{1}{2}\rangle^2\langle[2^{a}1^{b}]L_1|\}[2^{a}1^{b-1}]L\rangle^2$$

$$= \frac{[L_1]D([2^{a}1^{b-1}])}{[L]D([2^{a}1^{b}])}\langle d^{n-1}[2^{a}1^{b}]S_1|\}d^{n}[2^{a}1^{b-1}]S_1-\tfrac{1}{2}\rangle^2$$

$$\times \langle[2^{a}1^{b-1}]L|\}[2^{a}1^{b}]L_1\rangle^2$$

$$= \frac{[L_1]D([2^{a}1^{b-1}])}{[L]D([2^{a}1^{b}])}\frac{\langle d^{n-1}[2^{a}1^{b}]S_1|\}d^{n}[2^{a}1^{b-1}]S_1-\tfrac{1}{2}\rangle^2}{\langle d^{n-2}[2^{a}1^{b-1}]S_1-\tfrac{1}{2}|\}d^{n}[2^{a}1^{b}]S_1\rangle^2}$$

$$\times \langle d^{n-2}[2^{a}1^{b-1}]LS_1-\tfrac{1}{2}|\}d^{n-1}[2^{a}1^{b}]L_1S_1\rangle^2 \qquad \text{(II-13)}$$

where D(W) is the dimension of the representation W, and for $[w_1 w_2]$ of R_5 is given by[5]

$$D(w_1 w_2) = \frac{(w_1+w_2+2)(w_1-w_2+1)(2w_1+3)(2w_2+1)}{6} \qquad \text{(II-14)}$$

Terms like $\langle d^{n-1}[2^a 1^b]S_1 | \} d^n [2^a 1^{b-1}]S_1 - \frac{1}{2}\rangle$ appearing in (II-13) can be derived from Racah's[1] factorized cfp's given in the seniority scheme. In detail (and before modification rules have been applied to $[2^a 1^b]$)

$$\langle \ell^{n-1}[2^a 1^{b-1}]S-\tfrac{1}{2} | \} \ell^n [2^a 1^b]S\rangle^2 = \frac{(4\ell+4-n-2a-2s)(2a+4S+2)S}{2n(2\ell+2-2a-2S)(2S+1)}$$

$$\langle \ell^{n-1}[2^{a-1} 1^{b+1}]S+\tfrac{1}{2} | \} \ell^n [2^a 1^b]S\rangle^2 = \frac{(4\ell+4-n-2a-2S)2a(S+1)}{2n(2\ell+2-2a-2S)(2S+1)}$$

(II-15)

$$\langle \ell^{n-1}[2^{a+1} 1^{b-1}]S-\tfrac{1}{2} | \} \ell^n [2^a 1^b]S\rangle^2 = \frac{(n-2a-2S)(4\ell+6-2a)S}{2n(2\ell+2-2a-2S)(2S+1)}$$

$$\langle \ell^{n-1}[2^a 1^{b+1}]S+\tfrac{1}{2} | \} \ell^n [2^a 1^b]S\rangle^2 = \frac{(n-2a-2S)(4\ell+4-2a-4S)(S+1)}{(2n(2\ell+2-2a-2S)(2S+1)}$$

As an example the cfp $\langle d^2[2]^1\bar{L} | \} d^3[21]^2 L\rangle$ is calculated. (II-10) gives

$$\langle d^2[2]^1\bar{L} | \} d^3[21]^2 L\rangle^2 + \langle d^2[2]^1 L | \} d^3[1]^2 L\rangle^2$$

$$= \tfrac{1}{3} + \tfrac{2}{3}\langle d[1]^2 D | \} d^2[2]^1\bar{L}\rangle^2 (2\bar{L}+1) \begin{Bmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ 0 & \frac{1}{2} & \frac{1}{2} \end{Bmatrix} \begin{Bmatrix} \bar{L} & 2 & 2 \\ \bar{L} & 2 & L \end{Bmatrix}$$

But $\langle d^2[2]^1\bar{L}|\}d^3[1]^2L\rangle^2 = \delta(L,2)\frac{2\bar{L}+1}{20}\langle d[1]^2D|\}d^2[2]^1\bar{L}\rangle^2$

and all one to two particle cfp's are one. This gives the remarkably simple result

$$\langle d^2[2]^1\bar{L}|\}d^3[21]^2L\rangle^2 = \tfrac{1}{3} - \tfrac{1}{3}(2\bar{L}+1)\begin{Bmatrix}\bar{L} & 2 & 2\\ \bar{L} & 2 & L\end{Bmatrix} - \delta(L,2)\,\frac{2\bar{L}+1}{60}$$

The $U_5 \supset R_5$ dependence can now be factorized off by use of (II-15) and in this manner Table II, giving the $R_5 \supset R_3$ factorized cfp's, can be built up. This table, taken with (II-15), reciprocity, and particle-hole equivalence[1], viz.

$$\langle \ell^{n+1}\psi\{|\ell^n\psi'\rangle = (-1)^z\left\{\frac{(4\ell+2-n)\,[S'][L']}{(n+1)[S][L]}\right\}^{\frac{1}{2}} \times \langle \ell^{4\ell+1-n}\psi|\}\ell^{4\ell+2-n}\psi'\rangle$$

where $z = L+L'-\ell-S-S'+a+a'$, accounts for all one body cfp's of the d shell.

TABLE II

$R_5 \supset R_3$ Factorized cfp's

$\langle [1]D|\}[11]L\rangle^2$ $\quad 1$

$\langle [1]D|\}[2]L\rangle^2$ $\quad 1$

$\langle [11]\bar{L}|\}[11]L\rangle^2$ $\quad \frac{1}{3}(1-2(2\bar{L}+1)\begin{Bmatrix}\bar{L} & 2 & 2\\ \bar{L} & 2 & L\end{Bmatrix}$

$\langle [11]\bar{L}|\}[21]L\rangle^2$ $\quad \frac{2}{3}(1+(2\bar{L}+1)\begin{Bmatrix}\bar{L} & 2 & 2\\ \bar{L} & 2 & L\end{Bmatrix} - \delta(L,2)\,\frac{3}{10}\,(2\bar{L}+1)$

$\langle [2]\bar{L}|\}[21]L\rangle^2$ $\quad \frac{2}{3}(1-(2\bar{L}+1)\begin{Bmatrix}\bar{L} & 2 & 2\\ \bar{L} & 2 & L\end{Bmatrix} - \delta(L,2)\,\frac{1}{10}\,(2\bar{L}+1)$

$\langle [21]\bar{L}|\}[21]L\rangle^2$ $\quad \frac{3}{2}\Big[\frac{1}{4} - \frac{2\bar{L}+1}{18(2L+1)}\,(1+(2L+1)\begin{Bmatrix}L & 2 & 2\\ L & 2 & \bar{L}\end{Bmatrix})$

$$+ \frac{\delta(\bar{L}2)}{40}(25\delta(L0)-15-(-1)^L) + \frac{(2\bar{L}+1)}{12}\sum_{x=0}^{4}(-1)^x$$

$$\times\left(\begin{Bmatrix}\bar{L} & 2 & L\\ 2 & x & \bar{L}\\ x & 2 & 2\end{Bmatrix} + 2\begin{Bmatrix}x & 2 & 2\\ x & 2 & \bar{L}\end{Bmatrix}\begin{Bmatrix}x & 2 & \bar{L}\\ L & 2 & \bar{L}\end{Bmatrix}\right)\Big]$$

$\langle [21]\bar{L}|\}[22]L\rangle^2$ $\quad \frac{1}{4} + \Big(\delta(L,2)+\delta(L,4)\Big)\Big(\frac{2\bar{L}+1}{6}\begin{Bmatrix}L & 2 & 2\\ L & 2 & \bar{L}\end{Bmatrix} - \frac{2\bar{L}+1}{6(2L+1)}\Big)$

$$+ \frac{\delta(\bar{L}2)}{16}\Big((-1)^2\,\frac{1}{5} - \frac{39}{25} - 10\delta(L0) + \tfrac{2}{3}\delta(L2)$$

$$+ \tfrac{2}{3}\delta(L4)\Big) - \frac{2\bar{L}+1}{4}\sum_{x=0}^{4}(-1)^x$$

$$\Big[(2x+1)\begin{Bmatrix}\bar{L} & 2 & L\\ 2 & x & \bar{L}\\ x & 2 & 2\end{Bmatrix} - \begin{Bmatrix}\bar{L} & 2 & x\\ \bar{L} & 2 & L\end{Bmatrix}\Big]$$

Table II (contd)

$\langle [22]L|\}[22]L\rangle^2$

$$\tfrac{1}{2} + \frac{2\bar{L}+1}{8}\left(\frac{2}{25}(-1)^L - \frac{1}{2L+1} + \begin{Bmatrix} 2 & 2 & \bar{L} \\ 2 & L & \bar{L} \end{Bmatrix}\right.$$

$$\times \left(\frac{39}{50} - \frac{1}{10}(-1)^{\bar{L}}\right)$$

$$\left. + 26 \begin{Bmatrix} 2 & 6 & \bar{L} \\ 2 & L & \bar{L} \end{Bmatrix} \begin{Bmatrix} 6 & 2 & 4 \\ 6 & 2 & \bar{L} \end{Bmatrix} + 234 \begin{Bmatrix} 6 & 2 & \bar{L} \\ 2 & 4 & 6 \\ 4 & 2 & 2 \end{Bmatrix}\right)$$

$$+ \delta(L,2)\left(\delta(\bar{L}0)\tfrac{1}{8} - \delta(\bar{L}2)\frac{7}{48} - \delta(\bar{L}4)\frac{97}{240}\right.$$

$$+ \frac{2\bar{L}+1}{50}\left((-1)^{\bar{L}} - \frac{39}{5}\right) + \delta(\bar{L}4)\left(\frac{16}{5} - \frac{65}{34}\begin{Bmatrix} 2 & 4 & L \\ 2 & 4 & 6 \end{Bmatrix}\right.$$

$$\left.\left. - \frac{9}{8}\begin{Bmatrix} 4 & 2 & 2 \\ 4 & 2 & L \end{Bmatrix}\right) + \frac{2\bar{L}+1}{8}\sum_{x=0}^{4}(-1)^x$$

$$\left((2x+1)\begin{Bmatrix} L & 2 & \bar{L} \\ 2 & x & L \\ x & 2 & 2 \end{Bmatrix} - \begin{Bmatrix} L & 2 & x \\ L & 2 & \bar{L} \end{Bmatrix}\right) - \frac{2\bar{L}+1}{4}\sum_{x=0}^{4}\begin{Bmatrix} \bar{L} & 2 & x \\ \bar{L} & 2 & L \end{Bmatrix}$$

$$+ \frac{2\bar{L}+1}{4}\sum_{x=0}^{4}\sum_{y=0}^{4}\left[(-1)^{L+y}(2x+1)(2y+1)\begin{bmatrix} y & 2 & 2 & \bar{L} \\ x & 2 & L & y \\ \bar{L} & 2 & 2 & x \end{bmatrix}\right.$$

$$\left. - (-1)^{x+y}(2x+1)\begin{Bmatrix} \bar{L} & 2 & L \\ x & y & \bar{L} \\ y & 2 & 2 \end{Bmatrix}\right]$$

where $\begin{bmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{bmatrix}$ is a 12j symbol of the second kind[34].

4. Two Body cfp's

For simplicity, the discussion of two body cfp's will be illustrated by the two to four particle cfp only. The analogue to (II-10) is thus

$$\sum_{\beta} \langle d^2\alpha' L' S', d^2\alpha'' L'' S'' | \} d^4\beta L S \rangle \langle d^4\beta L S \{ | d^2\alpha_2 L_2 S_2, d^2\alpha_1 L_1 S_1 \rangle$$

$$= \frac{1}{6}\Big[\delta(\psi'\psi_1)\delta(\psi''\psi_2) + (-1)^{L_1+L_2-L+S_1+S_2-S}\delta(\psi'\psi_2)\delta(\psi''\psi_1)$$

$$- 4([L'][L''][L_1][L_2][S'][S''][S_1][S_2])^{\frac{1}{2}} \begin{Bmatrix} 2 & 2 & L' \\ 2 & 2 & L'' \\ L_1 & L_2 & L \end{Bmatrix} \begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & S' \\ \frac{1}{2} & \frac{1}{2} & S'' \\ S_1 & S_2 & S \end{Bmatrix}\Big] \qquad \text{(II-16)}$$

Hence, for example

$$\langle d^2[11]^3L_1, d^2[11]^3L_2 | \} d^4[1]^5D \rangle^2 = \frac{1}{6}\Big(1+(-1)^{L_1+L_2-L}\delta(L_1L_2) - 4[L_1][L_2]\begin{Bmatrix} 2 & 2 & L_1 \\ 2 & 2 & L_2 \\ L_1 & L_2 & L \end{Bmatrix}\Big)$$

However, the Kronecker products $[2^a1^b]\times[11]$ or $[2^a1^b]\times[2]$ unlike the one body case, introduce more than one "new" term, so by using (II-16) alone, all the two body cfp's cannot be built up. Thus one has the particularly simple result

$$\langle [11]^3L_1, [11]^3L_2 | \} [21]^3L \rangle^2 + \langle [11]^3L_1, [11]^3L_2 | \} [11]^2L \rangle^2 = \frac{1}{6}\left(1-(-1)^L\delta(L_1L_2)\right) \qquad \text{(II-17)}$$

with, however, two unknown cfp's on the left hand side.

We might hope to overcome this difficulty by building up one of the cfp's from one body cfp's using the well-known formula

$$\langle\psi\{|\tilde{\psi},\ell^2\alpha'L'S'\rangle = -\sum_{\bar{\psi}}([S'][L'][\bar{S}][L])^{\frac{1}{2}}(-1)^{x}\langle\psi\{|\bar{\psi}\rangle\langle\bar{\psi}\{|\tilde{\psi}\rangle \begin{Bmatrix} \frac{1}{2} & S' & \frac{1}{2} \\ S & \bar{S} & \tilde{S} \end{Bmatrix} \begin{Bmatrix} \ell & L' & \ell \\ L & \bar{L} & \tilde{L} \end{Bmatrix} \qquad \text{(II-18)}$$

where $x = S+\bar{S}+L+\bar{L}$.

To use (II-18), however, requires the knowledge of non-arbitrary relative phases between one-body cfp's, which the above derivations have not given. Other forms of (II-8), say

$$\sum_{\beta}\langle d^2\alpha'L'S',d^2\alpha''L''S''|\}d^4\beta LS\rangle\langle d^3\alpha_1L_1S_1,d|\}d^4\beta LS\rangle$$

$$= \tfrac{1}{2}(\langle d,d^2\alpha''L''S''|\}d^3\alpha_1L_1S_1\rangle(-1)^{L''+L_1+L'+S''+S_1+S'}$$

$$([L'][L_1][S'][S_1])^{\frac{1}{2}} \times \begin{Bmatrix} L & L_1 & 2 \\ 2 & L' & L'' \end{Bmatrix}\begin{Bmatrix} S & S_1 & \frac{1}{2} \\ \frac{1}{2} & S' & S'' \end{Bmatrix}$$

$$- \langle d^2\alpha'L'S',d|\}d^3\alpha_1L_1S_1\rangle(-1)^{L+L'+S+S'}([L''][L_1][S''][S_1])^{\frac{1}{2}}$$

$$\times \begin{Bmatrix} L'' & 2 & 2 \\ L_1 & L & L' \end{Bmatrix}\begin{Bmatrix} S'' & \frac{1}{2} & \frac{1}{2} \\ S_1 & S & S' \end{Bmatrix} \qquad \text{(II-19)}$$

can partly solve this problem, for by choosing $\alpha' = [11]$, $\alpha'' = [2]$, $\alpha_1 = [1]$ both the left and the right-hand side reduce to one term containing only known factors, viz.

$$\langle d^2[11]^3L', d^2[2]^1L'' | \} d^4[11]^3L \rangle \langle d^3[1]^4L_1 | \} d^4[11]^3L \rangle$$

$$= \langle d^2[11]^3L', d | \} d^3[1]^4L_1 \rangle (-1)^{L+L'} \left[\frac{(2L''+1)(2L_1+1)}{6}\right]^{\frac{1}{2}}$$

$$\times \begin{Bmatrix} L'' & 2 & 2 \\ L_1 & L & L' \end{Bmatrix}.$$

A formula of type (II-17) now gives $[11]\times[2] \rightarrow [21]$ and by use of reciprocity and tables of $U_5 \supset R_5$ two body cfp's[35] it is in principle possible to recover the cfp's $[11]\times[11] \rightarrow [22]$, $[2]$ and $[0]$.

In general though, there appears to be no systematic Redmond method for deriving all the two body cfp's that does not require firstly a resolution of the perennial phase problem.

5. Conclusions

The refinement to Redmond's formula can be applied systematically to the evaluation of one-body d shell cfp's but the method appears to break down for two body cfp's because of the awkwardness of the two body Kronecker product and difficulty with non-arbitrary phases. However,

in this case, and in the case of more general electronic and nuclear configurations, useful and in many cases pleasingly simple identities (c.f. (II-17)) can be derived which should allow existing techniques that translate from Redmond's formula, such as Nutter and Nielson's[31] projection method, to be carried out more directly and efficiently.

SECTION II

APPLICATIONS

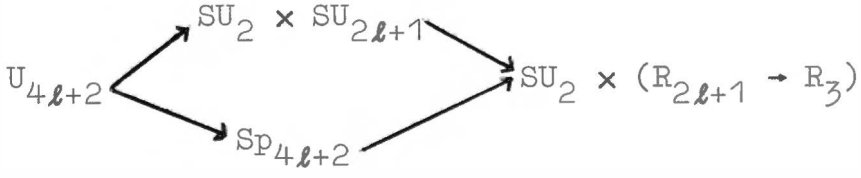
C H A P T E R I I I

QUASIPARTICLE FORMALISM AND ATOMIC SHELL THEORY

I. EQUIVALENT ELECTRONS[13]

1. Introduction

The theory of continuous groups has been used extensively both to classify eigenfunctions and interactions[1-3,5]. The orthonormal set of antisymmetrized eigenfunctions associated with an equivalent electron ℓ^N span the $\{1^N\}$ representation of the unitary group $U_{4\ell+2}$. The members of the set of eigenfunctions may be classified by considering their transformation properties under the operations of the various subgroups of $U_{4\ell+2}$. The chain of groups



(III-1)

may be used to completely distinguish the eigenfunctions in the d-shells (ℓ=2). If the exceptional Lie group G_2 is embedded in R_7 an almost complete classification of the eigenfunctions of the f-shell is possible[1]. For higher

values of ℓ the above classification scheme rapidly proves to give an inadequate number of classificating symbols to distinguish eigenfunctions associated with the same SL quantum numbers. Thus in the t^{13} configuration no distinction is possible among the 30598 ^{14}E states.

The chain of groups given in Eq. (III-1) sheds little light on relationships between the properties of configurations involving different numbers of electrons. This has led Judd[3] to consider the various subgroups of the group $U_{2^{4\ell+2}}$ which comprises the group of all unitary transformations among the $2^{4\ell+2}$ multielectron states of the ℓ-shell. He has shown that the chain of groups given in Eq. (III-1) may be replaced by the chain

$$U_{2^{4\ell+2}} \rightarrow R_{8\ell+5} \rightarrow R_{8\ell+4} \rightarrow SU_2^Q \times (Sp_{4\ell+2} \rightarrow SU_2 \times [R_{2\ell+1} \rightarrow R_3]). \qquad \text{(III-2)}$$

This chain of groups provides no additional classificatory symbols but does, through the introduction of the quasi-spin group SU_2^Q, display the N-dependence of the multi-electron states in a transparent manner.

The eigenfunctions of the ℓ-shell all transform according to the {1} representation of $U_{2^{4\ell+2}}$ which under restriction to the subgroup $R_{8\ell+5}$ goes down irreducibly into the basic spin representation $\Delta \equiv [(\frac{1}{2})^{4\ell+2}]$ of $R_{8\ell+5}$.

To obtain further classificatory symbols it is necessary to explore the subgroups of $R_{8\ell+5}$ that are alternatives to those of Eq. (III-2).

Judd[36] has shown that a much richer classification scheme is obtained decomposing the representation $\{1^N\}$ of $U_{4\ell+2}$ under the chain of groups

$$U_{4\ell+2} \rightarrow U^{\uparrow}_{2\ell+1} \times U^{\downarrow}_{2\ell+1} \rightarrow R^{\uparrow}_{3} \times R^{\downarrow}_{3} \rightarrow R_3 \qquad \text{(III-3)}$$

where the orbitally antisymmetrized eigenfunctions associated with electrons having their spins "up" ($m_s = +\frac{1}{2}$) transform under $U^{\uparrow}_{2\ell+1}$ and those with their spin "down" ($m_s = -\frac{1}{2}$) transform under $U^{\downarrow}_{2\ell+1}$. This chain of groups gives a complete classification of the eigenfunctions of the configurations ℓ^N up to $\ell = 3$ and for $\ell > 4$ proves much more successful in distinguishing states with the same SL quantum numbers than that of Eq. (III-1) though is of course no more successful in distinguishing the 30598 ^{14}E states of t^{13}.

These group structures have all been studied[3,36] by representing the Lie algebras in terms of the annihilation and creation operators of the method of second-quantization[6]. Armstrong and Judd[37] have recently showed that it is possible to develop an alternative classification scheme of the ℓ-shell by considering the properties of the basic tensor operators

$$\lambda_q^{(\ell)} = \frac{1}{\sqrt{2}}\left[a^+_{\frac{1}{2}q} + (-1)^{\ell-q}a_{\frac{1}{2}-q}\right]$$

$$\mu_q^{(\ell)} = \frac{1}{\sqrt{2}}\left[a^+_{\frac{1}{2}q} - (-1)^{\ell-q}a_{\frac{1}{2}-q}\right] \qquad \text{(III-4)}$$

$$\nu_q^{(\ell)} = \frac{1}{\sqrt{2}}\left[a^+_{-\frac{1}{2}q} + (-1)^{\ell-q}a_{-\frac{1}{2}-q}\right]$$

$$\xi_q^{(\ell)} = \frac{1}{\sqrt{2}}\left[a^+_{-\frac{1}{2}q} - (-1)^{\ell-q}a_{-\frac{1}{2}-q}\right]$$

where the subscripts to the annihilation and creation operators a and a^+ specify m_s and m_ℓ for an electron. Their results lead to the conclusion that the states of the ℓ-shell can be classified according to the scheme

$$R^{\uparrow}_{\lambda}(2\ell+1) \times R^{\uparrow}_{\mu}(2\ell+1) \times R^{\downarrow}_{\nu}(2\ell+1) \times R^{\downarrow}_{\xi}(2\ell+1) \qquad \text{(III-5)}$$

and its subgroups. There is no basic difficulty in extending their method to mixed configurations, see Chapter IV.

In this chapter I propose to demonstrate that the group structure suggested by Armstrong and Judd may be embedded in the group $R_{8\ell+5}$ in a natural manner which sheds considerable light on representation of atomic shells in the quasiparticle methods familiar in nuclear and superconductivity physics[38]. After careful consideration of the defining of the vacuum states appropriate to the quasiparticle operators a method for expanding the quasiparticle states in terms of the familiar determinantal

states is outlined. Finally, a method for calculating quasi-particle matrix elements is developed. The need for fractional parentage coefficients in calculating these matrix elements is entirely eliminated.

2. The Basic Group Structure

Armstrong and Judd[37] derived the group structure of Eq. (III-5) by showing that the coupled products,

$$\tfrac{1}{2}(\lambda^{(\ell)}\lambda^{(\ell)})^{(k)}_{q}, \quad -\tfrac{1}{2}(\mu^{(\ell)}\mu^{(\ell)})^{(k)}_{q}, \quad \tfrac{1}{2}(\nu^{(\ell)}\nu^{(\ell)})^{(k)}_{q}$$

$$\text{and} \quad -\tfrac{1}{2}(\xi^{(\ell)}\xi^{(\ell)})^{(k)}_{q},$$

with k <u>odd</u> form the generators of the rotation groups $R_\lambda(2\ell+1)$, $R_\mu(2\ell+1)$, $R_\nu(2\ell+1)$ and $R_\xi(2\ell+1)$ respectively. In this section I show that the group scheme of Armstrong and Judd is part of a larger structure of the form

$$R_{8\ell+5} \rightarrow R^{\uparrow}_{4\ell+2} \times R^{\downarrow}_{4\ell+2} \rightarrow R^{\uparrow}_{\lambda}(2\ell+1) \times R^{\downarrow}_{\mu}(2\ell+1) \times R^{\uparrow}_{\nu}(2\ell+1) \times R^{\downarrow}_{\xi}(2\ell+1), \qquad \text{(III-6)}$$

where as before the arrow ↑ is associated with eigenfunctions with $m_s = +\frac{1}{2}$ and the arrow ↓ with those associated with $m_s = -\frac{1}{2}$. The individual spin spaces may be further reduced by examining the subgroups of the $R_{2\ell+1}$ groups, e.g. in the spin-up space we have

$$R^{\uparrow}_{\lambda}(2\ell+1) \times R^{\uparrow}_{\mu}(2\ell+1) \rightarrow R^{\uparrow}_{\lambda}(3) \times R^{\uparrow}_{\mu}(3) \rightarrow R^{\uparrow}_{\lambda\mu}(3). \qquad \text{(III-7)}$$

Equations (III-4) can be re-expressed as

$$a^{+}_{\frac{1}{2}q} = \frac{1}{\sqrt{2}}(\lambda^{(\ell)}_{q} + \mu^{(\ell)}_{q}); \quad a_{\frac{1}{2}-q} = \frac{1}{\sqrt{2}}(-1)^{-q}(\lambda^{(\ell)}_{q} - \mu^{(\ell)}_{q})$$

$$a^{+}_{-\frac{1}{2}q} = \frac{1}{\sqrt{2}}(\nu^{(\ell)}_{q} + \xi^{(\ell)}_{q}); \quad a_{-\frac{1}{2}-q} = \frac{1}{\sqrt{2}}(-1)^{\ell-q}(\nu^{(\ell)}_{q} - \xi^{(\ell)}_{q}) \qquad \text{(III-8)}$$

Judd[3] has shown that for the ℓ-shell the $8\ell+4$ annihilation and creation operators, $a_{m_s m_\ell}$ and $a^{+}_{m_s m_\ell}$, together with their $(4\ell+2)(8\ell+3)$ distinct non-zero anticommutators close on the commutation algebra of the group $R_{8\ell+5}$ and thus the construction of the group $R_{8\ell+5}$ from the operators of Eq. (III-8) is self-evident.

Furthermore, the coupled products $\frac{1}{2}(\lambda^{(\ell)}\lambda^{(\ell)})^{(k)}_{q}$ and $-\frac{1}{2}(\mu^{(\ell)}\mu^{(\ell)})^{(k)}_{q}$ with k <u>odd</u>, together with the linear combinations $\frac{1}{2}(\lambda\mu)^{(k)}_{q} - (-1)^{k}\frac{1}{2}(\mu\lambda)^{(k)}_{q}$ for all k <u>even</u> or <u>odd</u> have the same commutation relations as those of the tensor operators $v^{(k)}_{q}(\ell_\lambda, \ell_\lambda)$ and $v^{(k)}_{q}(\ell_\mu, \ell_\mu)$ with k <u>odd</u> and $v^{(k)}_{q}(\ell_\lambda, \ell_\mu) + (-1)^{k} v^{(k)}_{q}(\ell_\mu, \ell_\lambda)$ with k <u>even</u> or <u>odd</u> and thus form the generators of the group[39] $R_{2(\ell_\lambda+\ell_\mu+1)}$, i.e. $R_{4\ell+2}$. Since the annihilation and creation operators used in constructing this group are all associated with $m_s = +\frac{1}{2}$ we designate this group as $R^{\uparrow}_{4\ell+2}$. The generators of the corresponding group $R^{\downarrow}_{4\ell+2}$ can likewise be readily

constructed from the annihilation and creation operators with $m_s = -\frac{1}{2}$. To develop the group structure further we must consider the group representations that arise in the classification of the multi-electron eigenfunctions.

3. The Basic Spin Representations

Having established the existence of the group chain $R_{8\ell+5} \rightarrow R^{\uparrow}_{4\ell+2} \times R^{\downarrow}_{4\ell+2}$ we show that the basic spin representation[23,40] Δ of $R_{8\ell+5}$, under restriction, decomposes into the conjugate spin representations $\Delta_1 = [\frac{1}{2} \cdots \frac{1}{2}]$, $\Delta_2 = [\frac{1}{2} \cdots -\frac{1}{2}]$ of the $R_{4\ell+2}$ groups in the following manner

$$\Delta \rightarrow (\Delta_1 + \Delta_2)^{\uparrow} \times (\Delta_1 + \Delta_2)^{\downarrow} \qquad \text{(III-9)}$$

where Δ_1 is to be associated with an <u>even</u> number of quasiparticles and Δ_2 with an <u>odd</u> number.

To establish the above result we first consider the group $R^{\uparrow}_{4\ell+2}$ and introduce the quasiparticle annihilation and creation operators

$$\beta^{(\ell)+}_{q} = \frac{1}{\sqrt{2}} (a^{+}_{\frac{1}{2}q} + (-1)^{\ell-q} a_{\frac{1}{2}-q}) = +\lambda^{(\ell)}_{q}$$

$$\beta^{(\ell)}_{q} = \frac{1}{\sqrt{2}} (a_{\frac{1}{2}q} + (-1)^{\ell-q} a^{+}_{\frac{1}{2}-q}) = (-1)^{\ell-q}\lambda^{(\ell)}_{-q}$$

$$\gamma^{(\ell)+}_{q} = \frac{1}{\sqrt{2}} (a^{+}_{\frac{1}{2}q} - (-1)^{\ell-q} a_{\frac{1}{2}-q}) = -(-1)^{\ell-q}\mu^{(\ell)}_{-q}$$

$$\gamma_q^{(\ell)} = \frac{1}{\sqrt{2}}\left(a^+_{\frac{1}{2}q} - (-1)^{\ell-q}\, a_{\frac{1}{2}-q}\right) = \mu_q^{(\ell)} \qquad \text{(III-10)}$$

all of which have $q > 0$. We then use these operators to define a normalized quasiparticle vacuum state $|\tilde{0}\rangle$ which is related to the normal particle vacuum state $|0\rangle$ by

$$|\tilde{0}\rangle = 2^{\ell/2} \prod_{q>0} \beta_q^{(\ell)} \prod_{q>0} \gamma_q^{(\ell)} |0\rangle. \qquad \text{(III-11)}$$

The above definition of the vacuum state has the necessary property that $\beta_q^{(\ell)}|\tilde{0}\rangle = 0$ for all the quasiparticle annihilation operators.

By using a natural extension of Judd's[5] operators

$$W_{\nu\mu} = \sum_{k,q} (-1)^{\ell-\nu}(1-(-1)^k) \begin{pmatrix} \ell & k & \ell \\ -\nu & q & \mu \end{pmatrix} v_q^{(k)}(\ell\ell)$$

we find that Weyl's commuting operators[41] for the group $R^{\uparrow}_{4\ell+2}$ are, in terms of the quasiparticle operators

$$H_q^{\lambda} = \tfrac{1}{2}[\beta_q^+, \beta_q], \qquad H_q^{\mu} = -\tfrac{1}{2}[\gamma_q^+ \gamma_q]$$

$$H_0^{\lambda\mu} = \tfrac{1}{2}(-1)^{\ell}[\beta_0, \gamma_0], \qquad \text{(III-12)}$$

where for convenience we now drop the quantum number ℓ of the electrons. H_q^{λ} gives eigenvalues $+\frac{1}{2}$ or $-\frac{1}{2}$ according to whether or not β_q^+ is, or is not, contained in the quasiparticle state $\beta_\mu^+ \ldots \beta_\tau^+ \gamma_\eta^+ \ldots \gamma_\rho^+ |\tilde{0}\rangle$ while H_q^{μ} gives eigenvalues $-\frac{1}{2}$ or $+\frac{1}{2}$ if γ_q^+ is, or is not, in the state.

Our definition of the quasiparticle vacuum makes it legitimate to include β_o or γ_o in the quasiparticle state, implying that if the state contains both β_o and γ_o, or neither of these, $H_o^{\lambda\mu}$ gives eigenvalues of $\frac{1}{2}(-1)^{\ell}$, while if the state contains only one of these the eigenvalues become $-\frac{1}{2}(-1)^{\ell}$.

The operators of $R^{\uparrow}_{4\ell+2}$, being coupled products of the λ's and μ's connect only states differing by two quasiparticles (or two ordinary particles) or none. It follows that if a state contains an <u>even</u> number of quasiparticles (including either β_o or γ_o) it transforms according to the representation $\Delta_1 = [\frac{1}{2} \ldots \frac{1}{2}]$ of $R^{\uparrow}_{4\ell+2}$, and if an <u>odd</u> number, according to the conjugate representation $\Delta_2 = [\frac{1}{2} \ldots -\frac{1}{2}]$. We note that our quasiparticle vacuum is proportional to

$$\prod_q (1+(-1)^{\ell-q} a^+_{-q} a^+_q)|0\rangle$$

i.e. contains an even number of real particles, and consequently if the quasiparticle number is even (odd), then the real particle number is even (odd).

Under the restriction $R_{4\ell+2} \rightarrow R_\lambda(2\ell+1) \times R_\mu(2\ell+1)$ both Δ_1 and Δ_2 decompose irreducibly into the product representations $\Delta^{\uparrow}_\lambda \times \Delta^{\uparrow}_\mu$ where Δ_λ and Δ_μ are the basic spin representations of the $R_{2\ell+1}$ rotation group. Similarly,

under restriction of $R^{\downarrow}_{4\ell+2}$ Δ_1 and Δ_2 decompose irreducibly into the product representation $\Delta^{\downarrow}_{\nu} \times \Delta^{\downarrow}_{\xi}$ of $R^{\downarrow}_{\nu}(2\ell+1) \times R_{\xi}(2\ell+1)$. The coupled product $\frac{1}{2}(\lambda^{(\ell)}\lambda^{(\ell)})^{(1)}_{q}$ supplies the generators of the group $R^{\uparrow}_{\lambda}(3)$ which is a subgroup of $R^{\uparrow}_{\lambda}(2\ell+1)$ and similarly $-\frac{1}{2}(\mu^{(\ell)}\mu^{(\ell)})^{(1)}_{q}$ gives the generators of $R^{\uparrow}_{\mu}(3)$. Thus we may write the complete group structure for describing the transformation of the ℓ-shell eigenfunctions in terms of the chain of groups

$$U_{2^{4\ell+2}} \rightarrow R_{8\ell+5} \rightarrow R^{\uparrow}_{4\ell+2} \times R^{\downarrow}_{4\ell+2} \rightarrow (R_{\lambda}(2\ell+1) \times R_{\mu}(2\ell+1))^{\uparrow}$$

$$\times (R_{\nu}(2\ell+1) \times R_{\xi}(2\ell+1))^{\downarrow} \rightarrow (R_{\lambda}(3) \times R_{\mu}(3))^{\uparrow}$$

$$\times (R_{\nu}(3) \times R_{\xi}(3))^{\downarrow} \rightarrow R^{\uparrow}_{\lambda\mu}(3) \times R^{\downarrow}_{\nu\xi}(3) \rightarrow R_{(3)} \rightarrow R_{(2)} \qquad \text{(III-13)}$$

If under the restriction $R_{2\ell+1} \rightarrow R_3$ the basic spin representation Δ decomposes into the representations of R_3 without repetitions then the chain of groups given in Eq. (III-13) will give a complete set of classificatory symbols to uniquely label all the eigenfunctions of the ℓ-shell. Methods of determining these branching rules have been discussed by Butler and Wybourne[40]. As noted by Armstrong and Judd, the classification is indeed unique for $\ell < 8$. It is interesting to note that even in the t-shell ($\ell = 14$) no representation of R_3 occurs more than 15 times in the

decomposition of the basic spin representation under $R_{29} \rightarrow R_3$.

It is evident from the nature of the chain of groups given in Eq. (III-13) that eigenfunctions constructed with these transformation properties will be characterized by well-defined L and M_L quantum numbers but will generally not correspond to a definite number of particles N or have accessible S and M_S quantum numbers. In trivial cases some identification may still be possible as may be seen when the quasiparticle states appropriate to the d-shell are expanded as linear combinations of determinantal states.

4. Quasiparticle and Determinantal States

The quasiparticle scheme is unlikely to be of calculational value if the quasiparticle states have to be first expanded as the linear combinations of the usual determinantal states. Rather we would like to calculate directly in the quasiparticle scheme. Nevertheless, it is useful in some applications to be able to make the transformation from quasiparticle states to determinantal states.

Consider the segment

$$R^{\uparrow}_{\lambda}(2\ell+1) \times R^{\uparrow}_{\mu}(2\ell+1) \rightarrow R^{\uparrow}_{\lambda}(3) \times R^{\uparrow}_{\mu}(3) \rightarrow R^{\uparrow}_{\lambda\mu}(3) \qquad \text{(III-14)}$$

of the group chain described by Eq. (III-13). Suppose under the restriction $R_{2\ell+1} \rightarrow R_3$ we have

$$\Delta_\varepsilon \rightarrow \Sigma\, g_{j_\varepsilon}[j_\varepsilon],$$

where g_{j_ε} is the number of times the $[j_\varepsilon]$ representation of $R_\varepsilon(3)$ arises in the decomposition, then the same branching rule holds for both $R^{\uparrow}_{\lambda}(2\ell+1)$ and $R^{\uparrow}_{\mu}(2\ell+1)$. Thus the problem of forming eigenfunctions where every electron in the ℓ-shell has $m_s = +\frac{1}{2}$ reduces to constructing eigenfunctions $|j_\lambda j_\mu; L_{\lambda\mu} M_{L_{\lambda\mu}}>^{\uparrow}$ for pseudo two-particle configurations $(j_\lambda j_\mu)^{\uparrow}$ where j_λ and j_μ will either be both half-integral or integral angular momentum.

For example, for the g-shell we find under $R_9 \rightarrow R_3$ $\Delta \rightarrow$ d+h and hence the LM_L states associated with all $m_s = +\frac{1}{2}$ will be the same as those arising in the three pseudo two-particle configurations $d_\lambda d_\mu$, $d_\lambda h_\mu$, $h_\lambda d_\mu$ and $h_\lambda h_\mu$.

We now wish to develop a systematic method for expanding the typical pseudo two-particle state $|j_\lambda j_\mu LM_L>^{\uparrow}$ as a linear combination of determinantal states. To do this we first construct a set of angular momentum ladder operators in the spaces of $R_\lambda(3)$ and $R_\mu(3)$ in terms of the quasi-particle annihilation and creation operators. These operators L^{λ}_{q} and L^{μ}_{q} must clearly be simply proportional to the coupled products $(\lambda^{(\ell)}\lambda^{(\ell)})^{(1)}_{q}$ and $(\mu^{(\ell)}\mu^{(\ell)})^{(1)}_{q}$ and in detail

$$L_0^{\lambda} = \sum_{q>0} qH_q^{\lambda} = \tfrac{1}{2}\sum_{q>0} q[\beta_q^+, \beta_q]$$

$$L_1^{\lambda} = -\sum_{q>0} (-1)^{\ell-q}[\tfrac{1}{2}(\ell+q)(\ell-q+1)]^{\frac{1}{2}}\lambda_q^{(\ell)}\lambda_{1-q}^{(\ell)}$$

$$= \sum_{q>0}[\tfrac{1}{2}(\ell+q)(\ell-q+1)]^{\frac{1}{2}}\beta_q^+\beta_{q-1} \qquad \text{(III-15a)}$$

and

$$L_0^{\mu} = -\sum_{q<0} qH_q^{\mu} = \tfrac{1}{2}\sum_{q>0} q[\gamma_q^+, \gamma_q]$$

$$L_{-1}^{\mu} = -\sum_{q<0} (-1)^{\ell-q}[\tfrac{1}{2}(\ell-q)(\ell+q+1)]^{\frac{1}{2}}\mu_q^{(\ell)}\mu_{-1-q}^{(\ell)}$$

$$= \sum_{q>0}[\tfrac{1}{2}(\ell+q)(\ell-q+1)]^{\frac{1}{2}}\gamma_q^+\gamma_{q-1} \qquad \text{(III-15b)}$$

The form of L_0 shows that the quasiparticle vacuum state is the state having the highest j_λ or j_μ and the lowest m_{j_λ} or highest m_{j_μ} in the $R_\lambda(3)$ and $R_\mu(3)$ spaces respectively. In obtaining these results we have required that the quasiparticle vacuum state $|\tilde{0}\rangle_\lambda$ in the λ space and $|\tilde{0}\rangle_\mu$ in the μ space may be coupled to yield the vacuum state $|\tilde{0}\rangle_\lambda|\tilde{0}\rangle_\mu \equiv |\bar{0}\rangle$ defined earlier for the $R^{\uparrow}_{4\ell+2}$ space. As a a result, we have, to within an inconsequential phase,

$$|\tilde{0}\rangle_\lambda = 2^{\ell/4}\prod_{q>0}\beta_q|0\rangle$$

and

$$|\tilde{0}\rangle \quad = \quad 2^{\ell/4} \prod_{q>0} \gamma_q |0\rangle .$$

Having constructed the angular momentum ladder operators it becomes a trivial matter to construct the angular momentum states $|j_\lambda m_\lambda\rangle$ and $|j_\mu m_\mu\rangle$ for highest j_λ and j_μ appropriate to the $R_\lambda(3)$ and $R_\mu(3)$ spaces in terms of an <u>even</u> number of quasiparticles (remembering to count a β_0 or a γ_0 if it occurs).

The angular momentum states for values of $j'_\lambda < j_\lambda$ or $j'_\mu < j_\mu$ may be constructed by requiring that the states $|j'_\lambda - m_{j'_\lambda}\rangle$ and $|j'_\mu m_{j'_\mu}\rangle$ be orthogonal to the states $|j_\lambda - m_{j'_\lambda}\rangle$ and $|j_\mu m_{j'_\mu}\rangle$ respectively and to any other states having the same $-m_{j'_\lambda}$ or $m_{j'_\mu}$, i.e. we construct an orthonormal set.

The states involving an <u>odd</u> number of quasiparticles in either space may be built up by applying the ladder operators to $\sqrt{2}\ \beta_0 |\tilde{0}\rangle$ and $\sqrt{2}\ \gamma_0 |\tilde{0}\rangle_\mu$ instead of to $|\tilde{0}\rangle_\lambda$ and $|\tilde{0}\rangle_\mu$. In each case the normalization is chosen so that $\langle j\text{-}j|j\text{-}j\rangle_\lambda$ and $\langle jj|jj\rangle_\mu$ are equal to $2^{-\ell/2}$.

As an example, consider the case of the d-shell where for $R_5 \rightarrow R_3$ we have $[\frac{11}{22}] \rightarrow \left[\frac{3}{2}\right]$. The proportionality constant required to recover the ladder operators is $\sqrt{10}$ and we have

$$L_0^\lambda = H_1^\lambda + 2H_2^\lambda \quad \text{and} \quad L_1^\lambda = \sqrt{2}\ \beta_2^+ \beta_1 + \sqrt{3}\ \beta_1^+ \beta_0, \qquad \text{(III-16a)}$$

and

$$L^{\mu}_{0} = -H^{\mu}_{1} - 2H^{\mu}_{2} \quad \text{and} \quad L^{\mu}_{-1} = \sqrt{2}\,\gamma^{+}_{2}\gamma_{0} + \sqrt{3}\,\gamma^{+}_{1}\gamma_{0} \tag{III-16b}$$

As a consequence for n_λ even (where n_λ is the number of quasiparticles in the λ space).

$$\left|\tfrac{3}{2}\ -\tfrac{3}{2}\right\rangle_\lambda = |\tilde{0}\rangle_\lambda, \qquad \left|\tfrac{3}{2}\ -\tfrac{1}{2}\right\rangle_\lambda = -\sqrt{2}\,\beta^{+}_{1}\beta_{0}|\tilde{0}\rangle_\lambda$$

$$\left|\tfrac{3}{2}\ \tfrac{1}{2}\right\rangle_\lambda = \sqrt{2}\,\beta^{+}_{2}\beta_{0}|\tilde{0}\rangle_\lambda \quad \text{and} \quad \left|\tfrac{3}{2}\ \tfrac{3}{2}\right\rangle_\lambda = \beta^{+}_{1}\beta^{+}_{2}|\tilde{0}\rangle_\lambda \tag{III-17a}$$

while for n_μ even in the μ space

$$\left|\tfrac{3}{2}\ \tfrac{3}{2}\right\rangle_\mu = |\tilde{0}\rangle_\mu, \qquad \left|\tfrac{3}{2}\ \tfrac{1}{2}\right\rangle_\mu = \sqrt{2}\,\gamma^{+}_{1}\gamma_{0}|\tilde{0}\rangle_\mu$$

$$\left|\tfrac{3}{2}\ -\tfrac{1}{2}\right\rangle_\mu = \sqrt{2}\,\gamma^{+}_{2}\gamma_{0}|\tilde{0}\rangle_\mu, \qquad \left|\tfrac{3}{2}\ -\tfrac{3}{2}\right\rangle_\mu = \gamma^{+}_{1}\gamma^{+}_{2}|\tilde{0}\rangle_\mu. \tag{III-17b}$$

Having constructed the states given in Eq. (III-17) we may perform a vector coupling to produce states characterized by the orbital quantum numbers L and M_L. For an even or odd total number of particles N

$$|j_\lambda j_\mu L_{\lambda\mu} M_{L_{\lambda\mu}}\rangle = \sum_{m_\lambda, m_\mu} \langle m_\lambda m_\mu | L_{\lambda\mu} M_{L_{\lambda\mu}}\rangle |j_\lambda m_\lambda, j_\mu m_\mu\rangle \tag{III-18}$$

where $\langle m_\lambda m_\mu | L_{\lambda\mu} M_{L_{\lambda\mu}}\rangle$ is the usual Clebsch-Gordon coefficient and

$$|j_\lambda m_\lambda, j_\mu m_\mu\rangle = \frac{(L_+^\lambda)^{j_\lambda - m_\lambda}(L_-^\mu)^{j_\mu + m_\mu}}{A \quad B} |j_\lambda m_{j_\lambda}, j_\mu - m_{j_\mu}\rangle \qquad \text{(III-19)}$$

with

$$A = \left[\frac{(2j_\mu)!(j_\mu - m_\mu)!}{(j_\mu + m_\mu)!}\right]^{\frac{1}{2}} \quad \text{and} \quad B = \left[\frac{(2j_\lambda)!(j_\lambda + m_\lambda)!}{(j_\lambda - m_\lambda)!}\right]^{\frac{1}{2}}.$$

If N is <u>even</u> and n_λ and n_μ are both even or odd then apart from an inconsequential phase

$$|j_\lambda - m_{j_\lambda}, j_\mu \; m_{j_\mu}\rangle = |\bar{0}\rangle$$

while if N is <u>odd</u> and n_λ and n_μ are of opposite parity

$$|j_\lambda - m_{j_\lambda}, j_\mu \; m_{j_\mu}\rangle = \sqrt{2}\,\beta_0|\bar{0}\rangle.$$

Using the above results for the particular case of the d-shell gives

$$|\Delta_1\left(\tfrac{3}{2}\right)_\lambda\left(\tfrac{3}{2}\right)_\mu F3\rangle = \beta_1^+\beta_2^+|\bar{0}\rangle = a_1^+a_2^+|0\rangle$$

and

$$|\Delta_2\left(\tfrac{3}{2}\right)_\lambda\left(\tfrac{3}{2}\right)_\mu F2\rangle = 2(\beta_2^+\beta_0 - \gamma_1^+\gamma_0\beta_1^+\beta_2^+)\beta_0|\bar{0}\rangle$$

$$= a_1^+a_2^+a_{-1}^+|0\rangle$$

while

$$|\Delta_2\left(\tfrac{3}{2}\right)_\lambda\left(\tfrac{3}{2}\right)_\mu D2\rangle' = 2(\beta_2^+\beta_0 + \gamma_1^+\gamma_0\beta_1^+\beta_2^+)\beta_0|\bar{0}\rangle$$

$$= -a_2^+|0\rangle,$$

where the creation operators a_q^+ are all associated with $m_s = +\frac{1}{2}$.

The construction of the states $|j_\nu j_\xi \; LM_L\rangle^\downarrow$ in the spin-down space proceeds in exactly the same manner except that the creation operators a_q^+ are now all associated with $m_s = -\frac{1}{2}$. The states constructed for the spin-up and spin-down spaces may be coupled by the usual vector-coupling method to give the final ℓ-shell eigenfunctions

$$|(j_\lambda j_\mu)L^\uparrow_{\lambda\mu}(j_\nu j_\xi)L^\downarrow_{\nu\xi}; LM_L\rangle$$

$$= \sum_{M_{L_{\lambda\mu}}, M_{L_{\nu\xi}}} \langle M_{L_{\lambda\mu}} \; M_{L_{\nu\xi}} | LM_L\rangle$$

$$|(j_\lambda j_\mu)L_{\lambda\mu} M_{L_{\lambda\mu}}\rangle^\uparrow |(j_\nu j_\xi)L_{\nu\xi} M_{L_{\nu\xi}}\rangle^\downarrow. \qquad \text{(III-20)}$$

These resultant eigenfunctions will not in general correspond to a definite number of particles but will however involve either <u>even</u> or <u>odd</u> numbers of particles.

It should be apparent from the preceding discussion that no significant complications arise when treating pseudo two-particle configurations where $j_\lambda \neq j_\mu$ or where j_λ and j_μ occur more than once in the decomposition of the basic spin representation of $R_{2\ell+1}$ to the group R_3.

5. Calculation of Matrix Elements

Any interaction may be expanded in terms of sums of products of tensor operators[5]. In the case of equivalent electron configurations ℓ^N the interactions may be expressed in terms of sums of products of the double tensor operators $\underset{\sim}{W}^{(Kk)}$ where

$$\underset{\sim}{W}^{(Kk)} = \sum_{i=1}^{N} \underset{\sim}{w}_i^{(Kk)}$$

and

$$\langle s\ell||w^{(Kk)}||s'\ell'\rangle = [(2K+1)(2k+1)]^{\frac{1}{2}}\delta(s,s')\delta(\ell\ell').$$

Judd[6] has shown that the double tensors $\underset{\sim}{W}^{(Kk)}$ may be related to coupled products of the usual annihilation and creation operators, viz.,

$$W^{(Kk)}_{\pi q} = -(a^+a)^{(Kk)}_{\pi q}. \qquad \text{(III-21)}$$

The annihilation and creation operators in Eq. (III-21) may be re-expressed in terms of the quasiparticle annihilation and creation operators using Eq. (III-8) and then decoupled to expose their spin dependence giving for k <u>odd</u>

$$W^{(K k)}_{\pi q} = -\tfrac{1}{2}[\langle s\tfrac{1}{2} s\tfrac{1}{2}|K\pi\rangle\{(\mu\nu)^{(k)}_q - (\lambda\xi)^{(k)}_q\} + \langle s-\tfrac{1}{2}\ s\tfrac{1}{2}|K\pi\rangle$$

$$\{(\nu\nu)^{(k)}_q - (\xi\xi)^{(k)}_q\} - \langle s\tfrac{1}{2}\ s-\tfrac{1}{2}|K\pi\rangle\{(\lambda\lambda)^{(k)}_q - (\mu\mu)^{(k)}_q\}$$

$$- \langle s-\tfrac{1}{2}\ s-\tfrac{1}{2}|K\pi\rangle\{(\nu\lambda)^{(k)}_q - (\xi\mu)^{(k)}_q\}] \qquad \text{(III-22a)}$$

and for k <u>even</u>

$$W^{(K k)}_{\pi q} = -\tfrac{1}{2}[\langle s\tfrac{1}{2}\ s\tfrac{1}{2}|K\pi\rangle\{(\mu\nu)^{(k)}_q - (\lambda\xi)^{(k)}_q + \delta(k,0)(2\ell+1)^{\frac{1}{2}}\}$$

$$+ \langle s-\tfrac{1}{2}\ s\tfrac{1}{2}|K\pi\rangle\{(\xi\nu)^{(k)}_q - (\nu\xi)^{(k)}_q + \delta(k,0)(2\ell+1)^{\frac{1}{2}}\}$$

$$- \langle s\tfrac{1}{2}\ s-\tfrac{1}{2}|K\pi\rangle\{(\mu\lambda)^{(k)}_q - (\lambda\mu)^{(k)}_q + \delta(k,0)(2\ell+1)^{\frac{1}{2}}\}$$

$$- \langle s-\tfrac{1}{2}\ s-\tfrac{1}{2}|K\pi\rangle\{(\xi\lambda)^{(k)}_q - (\nu\mu)^{(k)}_q + \delta(k,0)(2\ell+1)^{\frac{1}{2}}\}]$$

(III-22b)

All one-particle interactions can be expressed in terms of the quasiparticle operators of Eqs (III-22a) and (III-22b) and the relevant matrix elements evaluated in the λ, μ, ν, ξ spaces, i.e. for the pseudo-four particle configurations $j_\lambda j_\mu j_\nu j_\xi$ with states as defined in Eq. (III-20).

The two-particle interactions will involve terms of the form[42]

$$\sum_{i\neq j}[\underset{\sim}{W}_i^{(K_1k_1)}\ \underset{\sim}{W}_j^{(K_2k_2)}]^{(Kk)K}_{Q} = [\underset{\sim}{W}^{(K_1k_1)}\ \underset{\sim}{W}^{(K_2k_2)}]^{(Kk)K}_{Q}$$

$$- (-1)^{2\ell+2s+K+k}[(2K_1+1)(2K_2+1)(2k_1+1)(2k_2+1)]^{\frac{1}{2}}$$

$$\times \begin{Bmatrix} k_1 & k_2 & k \\ \ell & \ell & \ell \end{Bmatrix} \begin{Bmatrix} K_1 & K_2 & K \\ s & s & s \end{Bmatrix} \underset{\sim}{W}^{(Kk)K}_{Q}. \qquad \text{(III-23)}$$

For scalar interactions where $K = k = K = Q = 0$ Eq. (III-23) reduces to

$$\sum_{i\neq j}(\underset{\sim}{W}_i^{(Kk)}\cdot\underset{\sim}{W}_j^{(Kk)}) = \underset{\sim}{W}^{(Kk)}\cdot\underset{\sim}{W}^{(Kk)} - \left[\frac{(2K+1)^2(2k+1)^2}{(4\ell+2)}\right]^{\frac{1}{2}}\underset{\sim}{W}^{(oo)} \qquad \text{(III-24)}$$

where $K_1 = K_2$ and $k_1 = k_2$ and we drop the subscripts.

Having expressed the one- and two-particle interactions in terms of quasiparticle operators the matrix elements may be directly evaluated using the standard methods of tensor operators and angular momentum recoupling[5] and thus entirely eliminating the need for the fractional parentage coefficients that arise in the traditional evaluation of matrix elements.

The use of tensor operator methods requires the evaluation of the reduced matrix elements of the quasiparticle operators between quasiparticle states. The reduced matrix elements of the quasiparticle operators will be zero between states containing the same number of quasiparticles.

The reduced number of matrix elements may be generally evaluated by expanding a particular component of the operator, say $\lambda_0^{(\ell)}$, together with the states of the bra and ket in terms of ordinary annihilation and creation operators remembering that the states are orthogonal, though not usually orthonormal. For the particular case of maximum $j = j_M$ in the space under consideration a simple formula can be found, viz.,

$$\begin{aligned} \langle \Delta_1 j_M || A^{(\ell)} || \Delta_2 j_M \rangle &= \pm \langle \Delta_2 j_M || A^{(\ell)} || \Delta_1 j_M \rangle \\ &= \pm (-1)^{\ell+2j_M} [2^{\frac{1}{2}} \begin{pmatrix} j_M & \ell & j_M \\ j_M & 0 & -j_M \end{pmatrix}]^{-1} \\ &= \pm \frac{[(2j_M-\ell)!(2j_M+\ell+1)!/2]^{\frac{1}{2}}}{(2j_M)!} \end{aligned} \qquad \text{(III-25)}$$

where the + sign is taken if A is λ or ν and the - sign if A is μ or ξ. For example, we may readily deduce from Eq. (III-25) that

$$\langle \Delta_1 \tfrac{3}{2} || \lambda^{(2)} || \Delta_2 \tfrac{3}{2} \rangle = \sqrt{10}. \qquad \text{(III-26)}$$

The matrix elements of the Coulomb repulsion may be readily calculated in the quasiparticle scheme by first noting that for equivalent electron configurations ℓ^N we have[5]

$$\sum_{i>j} \frac{e^2}{r_{ij}} = e^2 \sum_k \frac{r_<^k}{r_>^{k+1}} \frac{(\ell||C^{(k)}||\ell)^2}{2k+1} \sum_{i\neq j} (\underset{\sim}{w}_i^{(ok)} \cdot \underset{\sim}{w}_j^{(ok)})$$

and from Eq. (III-24)

$$\sum_{i\neq j} (\underset{\sim}{w}_i^{(ok)} \cdot \underset{\sim}{w}_j^{(ok)}) = \underset{\sim}{W}^{(ok)} \cdot \underset{\sim}{W}^{(ok)} - \frac{(2k+1)}{(4\ell+2)^{\frac{1}{2}}} \underset{\sim}{W}^{oo}, \quad \text{(III-27)}$$

and then expressing the matrix elements of $\underset{\sim}{W}^{(ok)}$ in terms of the quasiparticle operators via Eq. (III-22b).

The scalar operator $W^{(oo)}_{oo}$ is proportional to the number operator[6] $\Sigma a^+_\tau a_\tau$ and for the d-shell in the "spin-up" space will have eigenvalues $N/(4\ell+2)^{\frac{1}{2}}$ where N is the number of particles since in this case every state corresponds to a definite number of particles. For more general cases the eigenvalues of $W^{(oo)}_{oo}$ will reflect the mixing of particle numbers in the quasiparticle state. This sometimes leads to a simple method for expanding the pseudo-particle states as linear combinations of the usual $|\ell^N SLM_S M_L\rangle$ states to within a phase.

As an example of the above, consider the states of the f-shell in the spin-up space. The states may be constructed in terms of pseudo-particles having 3 and 0 units of angular momentum since under $R_7 \rightarrow R_3$ we have $\Delta \rightarrow [3] + [0]$. Evaluation of the matrix element of $W^{(oo)}_{oo}$ for the S-states for an even number of f-electrons proceeds in the

pseudo-particle scheme as follows:

$$\langle \Delta_1(3)_\lambda(3)_\mu;SO|W^{(oo)}_{oo}|\Delta_1(3)_\lambda(3)_\mu;SO\rangle$$

$$= \frac{1}{\sqrt{2}}\langle \Delta_1(3)_\lambda(3)_\mu;SO|(\mu\lambda)^{(o)}_{o}|\Delta_1(3)_\lambda(3)_\mu;SO\rangle + \frac{\sqrt{14}}{4}$$

$$= \frac{1}{\sqrt{2}}\langle \Delta_1(3)_\lambda(3)_\mu;S||(\mu\lambda)^{(o)}||\Delta_1(3)_\lambda(3)_\mu;S\rangle + \frac{\sqrt{14}}{4}$$

$$= \frac{1}{\sqrt{2}}\begin{Bmatrix} 3 & 3 & 3 \\ 3 & 3 & 3 \\ 0 & 0 & 0 \end{Bmatrix}\langle \Delta_1(3)_\mu||\mu^{(3)}||\Delta_2(3)_\mu\rangle\langle \Delta_2(3)_\lambda||\lambda^{(3)}||\Delta_1(3)_\lambda\rangle$$

$$+ \frac{\sqrt{14}}{4}$$

$$= \frac{\sqrt{14}}{28},$$

and since we must necessarily have

$$|\Delta_1(3)_\lambda(3)_\mu;SO\rangle = a|f^4\ {}^5S\ M_S = 2M_L = 0\rangle + b|f^o\ {}^1S\ M_S$$

$$= 0\ M_L = 0\rangle$$

we find $a^2 = \frac{1}{8}$ and $b^2 = \frac{7}{8}$. Similarly, for an <u>odd</u> number of f-electrons,

$$|\Delta_2(3)_\lambda(3)_\mu;SO\rangle = a|f^3\ {}^4S\ M_S = \tfrac{3}{2}\ M_L = 0\rangle$$

$$+ b|f^7\ {}^8S\ M_S = \tfrac{7}{2}\ M_L = 0\rangle$$

where again $a^2 = \frac{1}{8}$ and $b^2 = \frac{7}{8}$. The above states will be

orthogonal to the states $|\Delta_1(0)_\lambda(0)_\mu;S0\rangle$ and $|\Delta_2(0)_\lambda(0)_\mu;S0\rangle$.

To summarize, the matrix elements of any interaction may be calculated in the quasiparticle formalism by following the steps, (1) Express the interaction in terms of sums of products of the tensor operators $\underset{\sim}{W}^{(Kk)}$; (2) Express the sums of products of the tensor operators $\underset{\sim}{W}^{(Kk)}$ as sums and products of the coupled products of the quasiparticle operators $(\underset{\sim}{\lambda}\underset{\sim}{\mu})^{(k)}$ etc.; (3) Calculate the matrix elements of the quasiparticle operators within the pseudo-four particle configuration $j_\lambda\ j_\mu\ j_\nu\ j_\xi$ evaluating the reduced matrix elements as required.

6. Conclusions

The establishment of the complete group chain in Eq. (III-13) sheds further light on the role of the quasiparticle formalism in atomic shell theory. The principal disadvantage of the quasiparticle scheme would seem to be the abandonment of the spin quantum numbers SM_S and the formation of eigenfunctions involving an indefinite number of particles.

The shortcomings of the quasiparticle formalism are partially compensated by the establishment of a remarkably rich classification scheme. Furthermore, the calculation

of matrix elements in the quasiparticle scheme requires little more than a knowledge of the theory of angular momentum recoupling coefficients and if combined with the powerful diagrammatic methods of Jucys et al.[34] becomes a trivial problem readily amenable to machine calculation without recourse to the usual coefficients of fractional parentage.

C H A P T E R I V

QUASIPARTICLE FORMALISM AND ATOMIC SHELL THEORY
II. MIXED CONFIGURATIONS[14]

1. Introduction

To date, the application of quasi-particle methods to mixed configurations has been treated by only one author, Feneuille[43], who considered the case of $(s+d)^N$. In this chapter I extend the methods and formalism of Ch. III to general mixed configurations. The relevant group structure becomes:

$$U_{2^{2\rho}} \rightarrow R_{4\rho+1} \rightarrow R^{\uparrow}_{2\rho} \times R^{\downarrow}_{2\rho} \rightarrow (R^{\lambda}_{\rho} \times R^{\mu}_{\rho})^{\uparrow} \times (R^{\xi}_{\rho} \times R^{\nu}_{\rho})^{\downarrow}$$

$$\rightarrow (R^{\lambda}_{3} \times R^{\mu}_{3})^{\uparrow} \times (R^{\xi}_{3} \times R^{\nu}_{3})^{\downarrow} \rightarrow R^{\lambda\mu\uparrow}_{3} \times R^{\xi\mu\downarrow}_{3} \rightarrow R_{3} \rightarrow R_{2} \qquad \text{(IV-1)}$$

where $\rho = \sum_i (2\ell_i+1)$ and the summation is taken over all orbitals characterizing the mixed configurations under study. Suitable linear combinations of fermion quasi-particle states are found forming bases for the spin representations Δ_1 or Δ_2 of $R_{2\rho}$ and Δ or one of Δ_1 or Δ_2 of R_{ρ} as ρ is odd or even. This linear combination allows us to find the decomposition of the vector representation $\{1\}$ of $U_{2^{2\rho}}$ under the group structure of Eq. (IV-1) and also to separate in a natural manner certain

multiplicities that arise at the R_3 level if three or more orbitals are under consideration. Finally, the $\underset{\sim}{W}^{(Kk)}(\ell\ell')$ tensor operators are expressed in the quasiparticle scheme and their matrix elements, which are shown to be generally both real and imaginary, are evaluated and as in the last Chapter, without the necessity of fractional parentage coefficients.

2. The Group Structure

In this section we establish the group structure specified in Eq. (IV-1). This is achieved by forming quasiparticle operators, $\lambda^{(\ell)}_q$ etc., as in Eq. (III-4) where now the ℓ quantum number can range over all the orbitals of the mixed configuration under consideration. The first two groups of the chain $(U_{2^{2\rho}} \rightarrow R_{4\rho+1})$ exist as a result of a self-evident extension of the results of Judd[3] and Feneuille[44] on the ordinary creation and annihilation operators which may easily be retrieved from

$$a^{(\ell)+}_{\frac{1}{2}q} = \frac{1}{\sqrt{2}}(\lambda^{(\ell)}_q + \mu^{(\ell)}_q) \text{ etc. (c.f. Eq. III-8).}$$

To prove the existence of the lower groups we must consider coupled products of the form $\frac{1}{2}(A^{\ell_i}B^{\ell_j})^{(K)}_Q$ where A and B are one of λ, μ, ξ, ν. We note that if $A \equiv B$ and

$\ell_i \equiv \ell_j$ this coupled product exists only for odd k and k = 0. These coupled products satisfy the commutation relations (all ℓ's assumed integral)

$$
\begin{aligned}
&[\tfrac{1}{2}(A^{\ell_1}{}_B{}^{\ell_2})^{(K_1)}_{Q_2}, \tfrac{1}{2}(C^{\ell_3}{}_D{}^{\ell_4})^{(K_2)}_{Q_2}] \\
&= \tfrac{1}{2}a_{BC}\delta(\ell_2,\ell_3)\delta(B,C)\sum_{K_3,Q_3}(-1)^{\ell_1+\ell_4+K_1+K_2+K_3-Q_3} \\
&[K_1,K_2,K_3]^{\frac{1}{2}} \begin{Bmatrix} K_1 & K_2 & K_3 \\ \ell_4 & \ell_1 & \ell_2 \end{Bmatrix} \begin{pmatrix} K_1 & K_2 & K_3 \\ Q_1 & Q_2 & -Q_3 \end{pmatrix} \tfrac{1}{2}(A^{\ell_1}{}_D{}^{\ell_4})^{(K_3)}_{Q_3} \\
&- \tfrac{1}{2}a_{AD}\delta(\ell_1,\ell_4)\delta(A,D)\sum_{K_3,Q_3}(-1)^{\ell_2+\ell_3-Q_3}[K_1,K_2,K_3]^{\frac{1}{2}} \\
&\begin{Bmatrix} K_1 & K_2 & K_3 \\ \ell_3 & \ell_2 & \ell_1 \end{Bmatrix} \begin{pmatrix} K_1 & K_2 & K_3 \\ Q_1 & Q_2 & -Q_3 \end{pmatrix} \tfrac{1}{2}(C^{\ell_3}{}_D{}^{\ell_4})^{(K_3)}_{Q_3} \\
&- \tfrac{1}{2}a_{DB}\delta(\ell_4,\ell_2)\delta(D,B)\sum_{K_3,Q_3}(-1)^{\ell_1+\ell_2+K_1+K_3-Q_3}[K_1,K_2,K_3]^{\frac{1}{2}} \\
&\begin{Bmatrix} K_1 & K_2 & K_3 \\ \ell_3 & \ell_1 & \ell_2 \end{Bmatrix} \begin{pmatrix} K_1 & K_2 & K_3 \\ Q_1 & Q_2 & -Q_3 \end{pmatrix} \tfrac{1}{2}(A^{\ell_1}{}_C{}^{\ell_3})^{(K_3)}_{Q_3} \\
&+ \tfrac{1}{2}a_{AC}\delta(\ell_1,\ell_3)\delta(A,C)\sum_{K_3,Q_3}(-1)^{\ell_2+\ell_3+K_2-Q_3}[K_1,K_2,K_3]^{\frac{1}{2}} \\
&\begin{Bmatrix} K_1 & K_2 & K_3 \\ \ell_4 & \ell_2 & \ell_1 \end{Bmatrix} \begin{pmatrix} K_1 & K_2 & K_3 \\ Q_1 & Q_2 & -Q_3 \end{pmatrix} \tfrac{1}{2}(D^{\ell_4}{}_D{}^{\ell_2})^{(K_3)}_{Q_3}, \qquad \text{(IV-2)}
\end{aligned}
$$

where a_{XY} is +1 if X = Y = λ or ξ, or -1 if X = Y = μ or ν.

If we now consider the operators like

$$(-1)^{(a+b)/2}(\tfrac{1}{2}(A^{\ell_1}B^{\ell_2})^{(K)}_{Q} - (-1)^{\ell_1-\ell_2+K}(\tfrac{1}{2}B^{\ell_2}A^{\ell_1})^{(K)}_{Q}$$

where a = 2 if A = λ or ξ, or a = +1 if A = μ or ν and similarly between b and B, we find the following commutation relation. (Note that $(-1)^{(a+b)/2}$ can be imaginary).

$$[(-1)^{(a+b)/2}\{\tfrac{1}{2}(A^{\ell_1}B^{\ell_2})^{(K_1)}_{Q_1} - (-1)^{\ell_A-\ell_B+K_1}\tfrac{1}{2}(B^{\ell_2}A^{\ell_1})^{(K_1)}_{Q_1}\},$$

$$(-1)^{(c+d)/2}\{\tfrac{1}{2}(C^{\ell_3}D^{\ell_4})^{(K_2)}_{Q_2} - (-1)^{\ell_C-\ell_D+K}\tfrac{1}{2}(D^{\ell_4}C^{\ell_3})^{(K_2)}_{Q_2}\}]$$

$$= \sum_{K_3Q_3}(-1)^{K_3-Q_3+\ell_1+\ell_4}[K_1,K_2,K_3]^{\frac{1}{2}}\begin{pmatrix}K_1 & K_2 & K_3\\ Q_1 & Q_2 & -Q_3\end{pmatrix}$$

$$\times\Big(\delta(\ell_2\ell_3)\delta(BC)(-1)^{K_1+K_2}\begin{Bmatrix}K_1 & K_2 & K_3\\ \ell_4 & \ell_1 & \ell_2\end{Bmatrix}$$

$$(-1)^{(a+d)/2}\{\tfrac{1}{2}(A^{\ell_1}D^{\ell_4})^{(K_3)}_{Q_3} - (-1)^{\ell_1-\ell_4+K_3}\tfrac{1}{2}(D^{\ell_4}A^{\ell_1})^{(K_3)}_{Q_3}\}$$

$$+ \delta(\ell_1\ell_4)\delta(AD)\begin{Bmatrix}K_1 & K_2 & K_3\\ \ell_3 & \ell_2 & \ell_1\end{Bmatrix}(-1)^{(b+c)/2}\{\tfrac{1}{2}(B^{\ell_2}C^{\ell_3})^{(K_3)}_{Q_3}$$

$$- (-1)^{\ell_2-\ell_3+K_3}\tfrac{1}{2}(C^{\ell_3}B^{\ell_2})^{(K_3)}_{Q_3}\} \qquad \text{(contd)}$$

$$- \delta(\ell_2\ell_4)\delta(BD)(-1)^{K_1}\begin{Bmatrix} K_1 & K_2 & K_3 \\ \ell_3 & \ell_1 & \ell_2 \end{Bmatrix} (-1)^{(a+c)/2} \{\tfrac{1}{2}(A^{\ell_1}C^{\ell_3})^{(K_3)}_{Q_3}$$

$$- (-1)^{\ell_1-\ell_3+K_3} \tfrac{1}{2}(C^{\ell_3}A^{\ell_1})^{(K_3)}_{Q_3}\} - \delta(\ell_1\ell_3)\delta(AC)(-1)^{(K_2)}$$

$$\begin{Bmatrix} K_1 & K_2 & K_3 \\ \ell_4 & \ell_2 & \ell_1 \end{Bmatrix} (-1)^{(b+d)/2} \{\tfrac{1}{2}(B^{\ell_2}D^{\ell_4})^{(K_3)}_{Q_3} - (-1)^{\ell_2-\ell_4+K_3}$$

$$\tfrac{1}{2}(D^{\ell_4}B^{\ell_2})^{(K_3)}_{Q_3}\}\Big) \qquad \text{(IV-3)}$$

This is, however, precisely the commutation relation of the

$$\overline{V}^{(k)}_q(\ell_1,\ell_2) = V^{(k)}_q(\ell_1,\ell_2) - (-1)^{\ell_1-\ell_2+k} V^{(k)}_q(\ell_2,\ell_1)$$

operators of Butler and Wybourne[45]. Moreover, they have shown that the set of operators $\overline{V}^{(k)}_q(\ell_i,\ell_i)$ with <u>odd</u> allowed k and $\overline{V}^{(k)}_q(\ell_i,\ell_j)$ for all ℓ_i,ℓ_j $(i<j)$ of a given configuration with all allowed k form the infinitesimal operators for the group R_ρ. Hence the set of operators

$$(-1)^a\{\tfrac{1}{2}(A^{\ell_i}A^{\ell_j})^{(K)}_Q - (-1)^{\ell_i-\ell_j+K}\tfrac{1}{2}(A^{\ell_j}A^{\ell_i})^{(K)}_Q\} \quad (\ell_i < \ell_j)$$

form the infinitesimal operators for the group R^A_ρ (taking

K odd if $\ell_i = \ell_j$), while this set, together with

$$(-1)^b\{\tfrac{1}{2}(B^{\ell_i}B^{\ell_j})^{(K)}_Q(-1)^{\ell_i-\ell_j+K}\ \tfrac{1}{2}(B^{\ell_j}B^{\ell_i})^{(K)}_Q\} \qquad (\ell_i < \ell_j)$$

where B is the other of the pair (λ,μ) or (ξ,ν), and

$$(-1)^{(a+b)/2}\{\tfrac{1}{2}(A^{\ell_i}B^{\ell_j})^{(K)}_Q - (-1)^{\ell_i-\ell_j+K}\ (B^{\ell_j}A^{\ell_i})^{(K)}_Q\}$$

form the infinitesimal operators of $R^{\uparrow}_{2\rho}$ if the pair is (λ,μ) or $R^{\downarrow}_{2\rho}$ if the pair is (ξ,ν). We note that this construction of R_ρ differs from Feneuille's treatment[43] for he constructs this group in the two orbital case essentially from the coupled products $(\lambda^{\ell_1}\lambda^{\ell_1})^{(K)}_Q$, $(\mu^{\ell_2}\mu^{\ell_2})^{(K)}_Q$ and $(\lambda^{\ell_1}\mu^{\ell_2})^{(K)}_Q$. The R_3 part of the group chain follows immediately by limiting the tensor ranks to one and zero.

3. The Weyl Selfcommuting Operators

At this stage we define quasiparticle creation and annihilation operators of the same form as in the last chapter, viz:

$$\beta^{(\ell)+}_{\pm\frac{1}{2}q} = \frac{1}{\sqrt{2}}\,(a^{+}_{\pm\frac{1}{2}q} + (-1)^{\ell-q}a_{\pm\frac{1}{2}-q}) \equiv \lambda^{(\ell)}_q \text{ or } \xi^{(\ell)}_q$$

$$(\beta^{(\ell)+}_{\pm\frac{1}{2}q})^{+} = \beta^{(\ell)}_{\pm\frac{1}{2}q} = \frac{1}{\sqrt{2}}\,(a_{\pm\frac{1}{2}q} + (-1)^{\ell-q}a_{\pm\frac{1}{2}-q})$$

$$\equiv (-1)^{\ell-q}\lambda^{(\ell)}_q \qquad \text{or} \qquad (-1)^{\ell-q}\xi^{(\ell)}_q.$$

$$\gamma^{(\ell)+}_{\pm\frac{1}{2}q} = \frac{1}{\sqrt{2}}\left(a_{\pm\frac{1}{2}q} - (-1)^{\ell-q}a^{+}_{\pm\frac{1}{2}-q}\right) \equiv -(-1)^{\ell-q}\mu^{(\ell)}_{-q}$$

$$\text{or} \qquad -(-1)^{\ell-q}\nu^{(\ell)}_{-q}$$

$$(\gamma^{(\ell)+}_{\pm\frac{1}{2}q})^{+} = \gamma^{(\ell)}_{\pm\frac{1}{2}q} = \frac{1}{\sqrt{2}}\left(a^{+}_{\pm\frac{1}{2}q} - (-1)^{\ell-q}a_{\pm\frac{1}{2}-q}\right)$$

$$\equiv \mu^{(\ell)}_{q} \qquad \text{or} \qquad \nu^{(\ell)}_{q},$$

all with $q > 0$. In analogy with the last chapter, the quasiparticle vacuum becomes

$$N \prod_{\ell}\prod_{q>0}\beta^{(\ell)}_{q}\prod_{\ell}\prod_{q>0}\gamma^{(\ell)}_{q}|0\rangle = |\bar{0}\rangle$$

where N is a normalization constant suitably chosen such that $\langle\bar{0}|\bar{0}\rangle = 1$. This definition of the vacuum satisfies $\beta^{(\ell)}_{q}|\bar{0}\rangle = 0$ for all ℓ and q as required.

In order to find the representation by which a quasiparticle state transforms we must first form the Weyl commuting operators[41], hereafter referred to as the H operators, for the groups $R_{2\rho}$ and R_{ρ}. Let us designate a configuration by $(\ell_1 + \ell_2 + \ldots + \ell_{2n})^N$ for an <u>even</u> number of orbitals, or by $(\ell_1 + \ell_2 + \ldots + \ell_{2n+1})^N$ for an <u>odd</u> number of orbitals, where ℓ_i and ℓ_j may be identical if they are associated with different principal quantum numbers.

Butler and Wybourne[45] have shown, in terms of this notation, that if $W^{\ell_i \ell_j}_{ab}$ is defined as

$$W^{\ell_i \ell_j}_{ab} = \sum_{k,q} (-1)^{\ell_i - a} [k]^{\frac{1}{2}} \begin{pmatrix} \ell_i & k & \ell_j \\ -a & q & b \end{pmatrix} \{ V^{(k)}_q(\ell_i, \ell_j) - (-1)^{\ell_i - \ell_j + k} V^{(k)}_q(\ell_j, \ell_i) \qquad \text{(IV-4)}$$

then the operators required for R_ρ are of the forms $W^{\ell_i \ell_i}_{a\,a}$ for all ℓ_i characterizing the configuration with all permissible a, and

$$(-1)^{\frac{\ell_{2i-1} + \ell_{2i} + 1}{2}} W^{\ell_{2i-1} \ell_{2i}}_{0\,0},$$

where i runs from 1 to n.

In the quasiparticle scheme we find for R^λ_ρ

$$W^{\ell\ell}_{aa} = \tfrac{1}{2}(-1)^{\ell - a} [\lambda^{(\ell)}_a, \lambda^{(\ell)}_{-a}] = \tfrac{1}{2}[\beta^{(\ell)+}_a, \beta^{(\ell)}_a]$$

and

$$(-1)^{\frac{\ell_x + \ell_y + 1}{2}} W^{\ell_x \ell_y}_{0\,0} = \tfrac{1}{2}(-1)^{\frac{\ell_x + 3\ell_y + 1}{2}} [\lambda^{(\ell_x)}_0, \lambda^{(\ell_y)}_0]$$

$$= \tfrac{1}{2}(-1)^{\frac{\ell_x - \ell_y + 1}{2}} [\beta^{(\ell_x)}_0, \beta^{(\ell_y)}_0]$$

while for R^μ_ρ

$$W^{\ell\ell}_{aa} = -\tfrac{1}{2}(-1)^{\ell-a}[\mu^{(\ell)}_{a}, \mu^{(\ell)}_{-a}] = -\tfrac{1}{2}[\gamma^{(\ell)+}_{a}, \gamma^{(\ell)}_{a}]$$

and

$$(-1)^{\frac{\ell_x+\ell_y+1}{2}} W^{\ell_x\ell_y}_{0\,0} = -\tfrac{1}{2}(-1)^{\frac{\ell_x+3\ell_y+1}{2}}[\mu^{(\ell_x)}_{o}, \mu^{(\ell_y)}_{o}]$$

$$= -\tfrac{1}{2}(-1)^{\frac{\ell_x-\ell_y+1}{2}}[\gamma^{(\ell_x)}_{o}, \gamma^{(\ell_y)}_{o}]$$

where $x = 2i-1$ and $y = 2i$ in each case.

The H operators for the group $R^{\uparrow}_{2\rho}$ are identical to those for R^{λ}_{ρ} and R^{μ}_{ρ} except for the case of an odd number of orbitals when we must add the operator

$$H^{\lambda\mu} = \tfrac{1}{2}[\lambda^{(\ell)}_{o}, \mu^{(\ell)}_{o}] = \tfrac{1}{2}(-1)^{\ell}[\beta^{(\ell)}_{o}, \gamma^{(\ell)}_{o}]$$

where $\ell \equiv \ell_{2n+1}$, i.e. ℓ is the single arbitrarily chosen unpaired orbital of the configuration. It now remains to find the eigenfunctions of the H operators.

4. Representations

A general eigenfunction for the H operators of R_ρ^λ takes the form

$$N \{....\} \prod_{i=1}^{n} \Big[\Big((-1)^{\frac{1-\ell_x}{2}} \beta_o^{(\ell_x)} \pm_x (-1)^{\frac{\ell_y}{2}} \beta_o^{(\ell_y)} \Big)$$

$$\pm_y \Big(\frac{1}{\sqrt{2}} \pm_x (-1)^{\frac{1-\ell_x+\ell_y}{2}} \sqrt{2}\, \beta_o^{(\ell_x)} \beta_o^{(\ell_y)} \Big) \Big] |\tilde{0}\rangle$$

$$= \{....\} \prod_{i=1}^{n} M^{\lambda}_{\pm_x, \pm_y} \qquad \text{(IV-5)}$$

where $\{....\}$ denotes an arbitrary product of β quasi-particle creation operators with non-zero subscripts apart from possibly $\beta_o^{\ell_{2n+1}}$ if the number of orbitals is odd (see Chapter III), i is defined as in Section 3, i.e. the product is being taken over pairs of orbitals, and the subscript to the $\pm$ signs means that signs with different subscripts are independent, as before N is a suitable normalizing constant and $|\tilde{0}\rangle$ is the vacuum for the R_ρ^λ group and is

$$\propto \prod_{\ell} \prod_{q>0} \beta_q^{(\ell)} |0\rangle .$$

The operation of $W_{aa}^{\ell\ell}$ on the eigenfunctions of Eq. (IV-5) yields eigenvalues of $+\frac{1}{2}$ or $-\frac{1}{2}$ depending on

whether $\beta_o^{(\ell)+}$ is or is not present in $\{....\}$ (see Chapter III), while operating with

$$(-1)^{\frac{\ell_x+\ell_y+1}{2}} W_{o\,o}^{\ell_x \ell_y}$$

gives eigenvalues $\pm_x \frac{1}{2}$. The corresponding eigenfunction for R_ρ^μ is

$$N \{....\} \prod_{i=1}^{n} \left[\left((-1)^{\frac{1-\ell_x}{2}} \gamma_o^{(\ell_x)} \pm_x (-1)^{\frac{\ell_y}{2}} \gamma_o^{(\ell_y)} \right) \right.$$

$$\left. \pm_y \left((\tfrac{1}{\sqrt{2}} +_x (-1)^{\frac{1-\ell_x+\ell_y}{2}} \sqrt{2}\, \gamma_o^{(\ell_x)} \gamma_o^{(\ell_y)} \right) \right] |\tilde{0}\rangle$$

$$= \{....\} \prod_{i=1}^{n} M_{\pm x, \pm y}^{\mu} \qquad \text{(IV-6)}$$

where now $W_{aa}^{\ell\ell}$ yields eigenvalues $-\frac{1}{2}$ or $+\frac{1}{2}$ dependong on whether $\gamma_o^{(\ell)+}$ is or is not present in $\{....\}$, while

$$(-1)^{\frac{\ell_x+\ell_y+1}{2}} W_{o\,o}^{\ell_x \ell_y}$$

gives eigenvalues $\pm_x (-1)^{\ell_x+\ell_y} \frac{1}{2}$.

It would appear that the quasiparticle states do indeed form a basis for a spin representation. However, if ρ is odd the dimension of the basic spin representation Δ of R_ρ is

$$2^{\sum_i^{2n+1} \ell_i + n} ,$$

with n defined as in Section 3, while the dimension of the conjugate spin representations of R_ρ for <u>ρ even</u> is

$$2^{\sum_i^{2n} \ell_i + n - 1}$$

It is clear from Eqs (IV-5) and (IV-6) that the number of eigenstates for R_ρ is

$$2^{\sum_i^{2n} \ell_i + 2n} ,$$

(for ρ <u>even</u>) or

$$2^{\sum_i^{2n+1} \ell_i + 2n}$$

(for ρ <u>odd</u>), i.e. 2^n greater than the dimension of the corresponding spin representations. This apparent discrepancy arises since the weight vector can be obtained in any of 2^n ways simply by allowing all combinations in the choice of sign labelled by y. To resolve this problem we consider the group $R_{2\rho}$.

A general eigenfunction for this group is of the form

$$N\{\ldots\}\prod_{i=1}^{n} M^{\lambda}_{(\pm x,\pm y)}\prod_{i=1}^{n} M^{\mu}_{(\pm x,\pm y)}|\bar{0}\rangle$$

where $\{\ldots\}$ is now a product of β and γ quasiparticle creation operators and with the possible inclusion of $\beta_o^{(\ell_{2n+1})}$ and $\gamma_o^{(\ell_{2n+1})}$. This is equal to

$$N\{\ldots.\}\prod_{i=1}^{n} M^{\lambda}_{(\pm x,\pm y)}M^{\mu}_{(\pm x,\pm y)}|\bar{0}\rangle$$

to within a phase since any two non-equivalent M's anti-commute. We now look at a typical term $M^{\lambda}_{(\pm x,\pm y)}$, $M^{\mu}_{(\pm x,\pm y)}$ which, expanded in full, is:

$$(-\tfrac{1}{2}\pm_{x_\mu}(-1)^{\frac{1-\ell_x+\ell_y}{2}}\beta_o^{(\ell_x)}\beta_o^{(\ell_y)}\pm_{x_\lambda}(-1)^{\frac{1-\ell_x+\ell_y}{2}}\beta_o^{(\ell_y)}\beta_o^{(\ell_x)}\pm_{x_\lambda}\pm_{x_\mu}$$

$$\pm_{y_\mu}\frac{1}{\sqrt{2}}\Big((-1)^{\frac{1-\ell_x}{2}}\beta_o^{(\ell_x)}\mp_{x_\mu}(-1)^{\frac{2+\ell_y}{2}}\beta_o^{(\ell_y)}\pm_{x_\lambda}(-1)^{\frac{\ell_y}{2}}\beta_o^{(\ell_y)}$$

$$\pm_{x_\lambda}\pm_{x_\mu}(-1)^{\frac{1-\ell_x}{2}}\beta_o^{(\ell_x)}\Big)$$

$$\pm_{y_\lambda}\frac{1}{\sqrt{2}}\Big((-1)^{\frac{1-\ell_x}{2}}\beta_o^{(\ell_x)}\pm_{x_\lambda}(-1)^{\frac{\ell_y}{2}}\beta_o^{(\ell_y)}\mp_{x_\mu}(-1)^{\frac{2+\ell_y}{2}}\beta_o^{(\ell_y)}$$

$$\pm_{x_\lambda}\pm_{x_\mu}(-1)^{\frac{1-\ell_x}{2}}\beta_o^{(\ell_x)}\Big)$$

$$\pm_{y_\lambda}\pm_{y_\mu}\Big(\tfrac{1}{2}\mp_{x_\mu}(-1)^{\frac{1-\ell_x+\ell_y}{2}}\beta_o^{(\ell_x)}\beta_o^{(\ell_y)}\pm_{x_\lambda}(-1)^{\frac{1-\ell_x+\ell_y}{2}}\beta_o^{(\ell_x)}\beta_o^{(\ell_y)}$$

$$\pm_{x_\lambda}\pm_{x_\mu}\tfrac{1}{2}\Big)$$

where for instance $\pm_{x_\lambda}\pm_{x_\mu}$ is + if x_λ and x_μ have the same sign and minus if their sign is different. We justify replacement of any $\gamma_o^{(\ell)}$ by $\beta_o^{(\ell)}$ by noting that

$$\gamma_o^{(\ell)}|\bar{0}\rangle = (N\prod_{\ell}\prod_{q>0}\beta_o^{(\ell)}\prod_{\ell}\prod_{q>0}\gamma_q^{(\ell)})\gamma_o^{(\ell)}|0\rangle$$

$$= (N\prod_{\ell}\prod_{q>0}\beta_q^{(\ell)}\prod_{\ell}\prod_{q>0}\gamma_q^{(\ell)})\frac{1}{\sqrt{2}}a_o^{(\ell)+}|0\rangle$$

$$= (N\prod_{\ell}\prod_{q>0}\beta_q^{(\ell)}\prod_{\ell}\prod_{q>0}\gamma_q^{(\ell)})\beta_o^{(\ell)}|0\rangle = \beta_o^{(\ell)}|\bar{0}\rangle$$

Clearly the above expression vanishes for certain sign choices, e.g. $x_\lambda = +1$, $y_\lambda = +1$, $x_\mu = +1$, $y_\mu = -1$. In fact if we choose $x_\lambda = +1$, $y_\lambda = +1$ then the only μ sign choices compatible (i.e. giving non-vanishing states) are $x_\mu = +1$, $y_\mu = +1$ and $x_\mu = -1$, $y_\mu = -1$, which are in turn compatible only with the original choice, and $x_\lambda = -1$, $y_\lambda = -1$. If we chose to start with a different sign

choice, our compatible set of sign choices, although different, will give the same quasiparticle states, to within a phase. As a consequence we see that at the R_ρ level we cannot make random choices in the sign labelled y_λ at the risk of throwing up a vanishing state at the $R_{2\rho}$ level. restricting ourselves then to some compatible set of sign choices, we see that we have

$$2^{\sum_i^{2n} \ell_i + 2n} \quad \text{or} \quad 2^{\sum_i^{2n+1} \ell_i + 2n+1}$$

states for $R_{2\rho}$,(as ρ <u>even</u> or <u>odd</u>) which is just the sum of the dimensions of Δ_1 and Δ_2 of $R_{2\rho}$, and

$$2^{\sum_i^{2n} \ell_i + n}$$

states (ρ <u>even</u>), or

$$2^{\sum_i^{2n+1} \ell_i + n}$$

(ρ <u>odd</u>) states at the R_ρ level as required.

Since the group operators, being coupled products of quasiparticle operators, connect only states differing by two or zero particles we see by considering the action of the H operators on a typical eigenstate that the set of

eigenstates in the λ-space (and similarly for the μ-space) form a basis for the spin representation Δ^{λ} or one of $\Delta_1^{\lambda}, \Delta_2^{\lambda}$ for the group R_{ρ}^{λ} according as ρ is odd or even, i.e. whether there is an odd or even number of orbitals. Moreover, they also form a basis for either the $\Delta^{\uparrow}{}_1$ or $\Delta^{\uparrow}{}_2$ spin representations of $R_{2\rho}^{\uparrow}$ where the parity of the particle number associated with $\Delta^{\uparrow}{}_1$ is the parity of n defined above and vice-versa for $\Delta^{\uparrow}{}_2$. For instance, this means that for the one orbital case (n=0) $\Delta^{\uparrow}{}_1$ is associated with an even number of particles and $\Delta^{\uparrow}{}_2$ is, with an odd number, as in Chapter III. The opposite is the case for two orbitals.

5. Branching Rules

We now show that the spin representation Δ of $R_{4\rho+1}$ decomposes as $(\Delta_1 + \Delta_2)^{\uparrow} \times (\Delta_1 + \Delta_2)^{\downarrow}$ under restriction to $R_{2\rho}^{\uparrow} \times R_{2\rho}^{\downarrow}$ and upon restriction to $R_{\rho}^{\lambda} \times R_{\rho}^{\mu}$, $\Delta_1^{\uparrow}$ and $\Delta_2^{\uparrow}$ decompose to $\Delta^{\lambda} \times \Delta^{\mu}$ if ρ is odd (number of orbitals odd) or as $\Delta_m^{\uparrow} \rightarrow \Delta_m^{\lambda} \times \Delta_2^{\mu} + \Delta_2^{\lambda} \times \Delta_m^{\mu}$ for ρ even where m' = 2 or 1 as m = 1 or 2. Further, upon restricting R_{ρ} to R_3 we show that we get a minimum multiplicity of 2^{n-1} or 2^n depending on whether n is even or odd. These duplicated R_3 representations can be separated in a natural manner.

The first branching rule is a direct consequence of the analysis of Section 4, i.e. that the representations Δ_1 and Δ_2 (spin up or down) are associated one with all possible states containing an even number of particles and one with all possible states containing an odd number of particles. Restricting the H operators to those of R_ρ clearly results in $\Delta_1^\uparrow$ and $\Delta_2^\uparrow$ decomposing to $\Delta^\lambda \times \Delta^\mu$ for ρ odd, but for ρ even a closer scrutiny is probably necessary. To this end we consider a set of eigenfunctions $\psi_{\Delta_m^{a \text{ or } b}}$ of $R_\rho^\uparrow$, where the subscript $\Delta_m^{a \text{ or } b}$ defines the representation by which the ψ's transform; Δ_1 if $m = 1$, Δ_2 if $m = 2$, and where $\psi_{\Delta_m^a}$ is defined as being that subset of ψ_{Δ_m} that has an even number of $-\frac{1}{2}$ eigenvalues under the H operators of R_ρ^λ, i.e. a restricted set of the H operators of $R_{2\rho}^\uparrow$. Similarly, $\psi_{\Delta_m^b}$ is that subset having an odd number of $-\frac{1}{2}$ eigenvalues under the H operators of R_ρ^λ. However, since the H operators of $R_{2\rho}^\uparrow$ for ρ even are just the H operators of R_ρ^λ and R_ρ^μ, (Section 3) then the set of H operators of R_ρ^μ must give an even (odd) number of $-\frac{1}{2}$'s if $m = 1$ ($m = 2$) when acting on the set $\psi_{\Delta_m^a}$ and an odd (even) number of $-\frac{1}{2}$'s if $m = 1$ ($m = 2$) when acting on the set $\psi_{\Delta_m^b}$. Thus $\psi_{\Delta_m^a}$ must transform, by definition, as $\psi_{\Delta_1^a}$ (the subscript to ψ now refers to the R_ρ^λ group) and as $\psi_{\Delta_m^\mu}$ under R_ρ^μ, i.e. as

$\psi_{\Delta_1^\lambda}\psi_{\Delta_m^\mu}$ while $\psi_{\Delta_m^b}$ must transform as $\psi_{\Delta_2^\lambda}$, by definition, and as $\psi_{\Delta_m^\mu,}$, i.e. $\psi_{\Delta_m^b}$ transforms as $\psi_{\Delta_2^\lambda}\psi_{\Delta_m^\mu,}$. Hence the set of functions ψ_{Δ_m}, being, by definition, $\psi_{\Delta_m^a} \cup \psi_{\Delta_m^b}$ must transform as

$$\psi_{\Delta_1^\lambda}\psi_{\Delta_m^\mu} + \psi_{\Delta_2^\lambda}\psi_{\Delta_m^\mu,},$$

i.e., we have established the branching rule under

$$R^{\uparrow}_{2\rho} \to R^{\lambda}_{\rho} \times R^{\mu}_{\rho} \quad \text{as} \quad \Delta_m^{\uparrow} \to \Delta_1^\lambda \times \Delta_m^\mu + \Delta_2^\lambda \times \Delta_m^{\mu,}.$$

It is interesting to note that for ρ even the $R^{\uparrow}_{2\rho}$ spin representation label becomes redundant in that this branching rule shows that the specification of the R^{λ}_{ρ} and R^{μ}_{ρ} label determines it. This is implicit in Feneuille's work[43].

6. Duplicated R_3 Representations

Upon finally restricting R_ρ to R_3 we note that since $\underset{\sim}{L} \propto \sum_{\ell} W^{(01)}(\ell\ell)$ we are restricting the set of transformations in such a manner that only the H's that do not mix the ℓ's (i.e. ${}^{\lambda}H^{\ell\ell}_{aa}$) remain (c.f. Chapter III and Section 5), since $L_0 = \sum_{\ell} \sum_{a>0} a\,{}^{\lambda}H^{\ell\ell}_{aa}$ for R^{λ}_{ρ}. We consider now that subset of the eigenfunctions forming a basis for Δ_1 (or Δ_2) for R^{λ}_{ρ} (ρ even) such that any wave function belonging to the set has $+\frac{1}{2}$ eigenvalues for $H^{\ell\ell}_{aa}$. On restriction to R_3 the eigenvalue of L_0 when acting upon any of these eigenfunctions will take its maximum value, equal to the maximum $L = L_M$ in the $R_\rho \rightarrow R_3$ branching rule. In fact,

$$L_M = \sum_{\ell} \sum_{a>0}^{\ell} \tfrac{1}{2}a = \tfrac{1}{4} \sum_{\ell} \ell(\ell+1).$$

However, since we have n H's that mix the ℓ's and their eigenvalues when acting on the above subset of wavefunctions are unrestricted we can see that this subset contains 2^{n-1} eigenfunctions. Consequently, under $R_\rho \rightarrow R_3$ we have $\Delta_1 \rightarrow 2^{n-1} L_M + \ldots$. A similar analysis for ρ odd shows that $\Delta \rightarrow 2^n L_M + \ldots$. Thus the multiplicity of the L_M representation of R_3 is 2^{n-1} (ρ even) or 2^n (ρ odd) and the multiplicity for any smaller allowed L will be an integral multiple of 2^{n-1} or 2^n. e.g. for $(s+p+d)^N$, under

$R_9 \rightarrow R_3$ we have $[\frac{1}{2}\ \frac{1}{2}\ \frac{1}{2}\ \frac{1}{2}] \rightarrow 2P + 2D$.

Fortunately, in this case, we have available a natural separation of duplicated R_3 representations amounting essentially to specifying, in addition to the R_ρ spin representation label, an R_ρ weight label. A state will then be labelled by a $R_{2\rho}$ and R_ρ spin representation label, a R_3 label and a n-vector Γ specifying the eigenvalues of the state under the H's that mix the ℓ's. Thus, for instance, the two D states of $(s+p+d)^N$ would be labelled as $|\Delta_a^{\uparrow}\Gamma = \pm\frac{1}{2}\ D\rangle$. (There being no R_ρ label needed here since it adds no new information).

7. Operators and Matrix Elements

As for equivalent electrons, any interaction can be written as sums of products of the tensor operators,

$$\underline{W}^{(Kk)}(\ell_A\ell_B) = \sum_{i=1}^{N} \underline{w}_i^{(Kk)}(\ell_A\ell_B) \quad \text{where}$$

$$\langle s\ell_A||w^{(Kk)}(\ell_B\ell_C)||s'\ell_D\rangle = [K,k]^{\frac{1}{2}}\delta(s,s')\delta(\ell_A\ell_B)\ \ell_B\ell_C).$$

Two particle interactions will involve terms of the form

$$\sum_{i\neq j}[\underset{\sim}{w}_i^{(K_1k_1)}(\ell_A,\ell_B)\underset{\sim}{w}_j^{(K_2k_2)}(\ell_C,\ell_D)]^{(Kk)}\,\overline{\overline{K}}_Q$$

$$= [\underset{\sim}{W}^{(K_1k_1)}\underset{\sim}{W}^{(K_2k_2)}]^{(Kk)}\,\overline{\overline{K}}_Q$$

$$- \delta(\ell_B,\ell_C)(-1)^{k+K+\ell_A+\ell_D+2s}[K_1,K_2,k_1,k_2]^{\frac{1}{2}}\begin{Bmatrix} k_2 & k & k_1 \\ \ell_A & \ell_B & \ell_D \end{Bmatrix}$$

$$\begin{Bmatrix} K_2 & K & K_1 \\ s & s & s \end{Bmatrix}(\underset{\sim}{W}^{(Kk)}(\ell_A\ell_D))\overline{\overline{K}}_Q$$

Morrison[46] has shown that $W^{(Kk)}_{\pi q}(\ell_A\ell_B)$ can be written in terms of coupled products of annihilation and creation operators as:

$$W^{(Kk)}_{\pi q}(\ell_A\ell_B) = -(a^{\ell_A\dagger}\underset{\sim}{a}^{\ell_B})^{(Kk)}_{\pi q}$$

where

$$\underset{\sim}{a}^{\ell_B}_{m_s m_\ell} = (-1)^{s+\ell_B-m_s-m_\ell}a_{-m_s-m_\ell}.$$

We may then express $W^{(Kk)}_{\pi q}(\ell_A\ell_B)$ in terms of our quasiparticle operators as was done in Chapter III giving:

$$W^{(K k)}_{\pi q}(\ell_A \ell_B) = -\tfrac{1}{2}\Big[\langle s\tfrac{1}{2} s\tfrac{1}{2} | K\pi\rangle \{ (\lambda^{\ell_A} \nu^{\ell_B})^{(k)}_{q} - (\mu^{\ell_A} \nu^{\ell_B})^{(k)}_{q}$$

$$+ (\mu^{\ell_A} \nu^{\ell_B})^{(k)}_{q} - (\lambda^{\ell_A} \xi^{\ell_B})^{(k)}_{q} + \delta(k,0)\delta(\ell_A,\ell_B)[\ell_A]^{\frac{1}{2}} \}$$

$$+ \langle s-\tfrac{1}{2} s\tfrac{1}{2} | K\pi\rangle \{ (\nu^{\ell_A} \nu^{\ell_B})^{(k)}_{q} - (\xi^{\ell_A} \xi^{\ell_B})^{(k)}_{q} + (\xi^{\ell_A} \nu^{\ell_B})^{(k)}_{q}$$

$$- (\nu^{\ell_A} \xi^{\ell_B})^{(k)}_{q} + \delta(k,0)\delta(\ell_A,\ell_B)[\ell_A]^{\frac{1}{2}} \}$$

$$- \langle s\tfrac{1}{2} s-\tfrac{1}{2} | K\pi\rangle \{ (\lambda^{\ell_A} \lambda^{\ell_B})^{(k)}_{q} - (\mu^{\ell_A} \mu^{\ell_B})^{(k)}_{q} + (\mu^{\ell_A} \lambda^{\ell_B})^{(k)}_{q}$$

$$- (\lambda^{\ell_A} \mu^{\ell_B})^{(k)}_{q} + \delta(k,0)\delta(\ell_A \ell_B)[\ell_A]^{\frac{1}{2}} \}$$

$$- \langle s-\tfrac{1}{2} s-\tfrac{1}{2} | K\pi\rangle (\nu^{\ell_A} \lambda^{\ell_B})^{(k)}_{q} - (\xi^{\ell_A} \mu^{\ell_B})^{(k)}_{q} - (\xi^{\ell_A} \lambda^{\ell_B})^{(k)}_{q}$$

$$- (\nu^{\ell_A} \mu^{\ell_B})^{(k)}_{q} + \delta(k,0)\delta(\ell_A \ell_B)[\ell_A]^{\frac{1}{2}} \} \Big] \qquad \text{(IV-7)}$$

For $\ell_A \equiv \ell_B$ this formula splits into two disjoint parts for k even and k odd, as in Chapter 3.

It is clear that, as in Chapter 3, any quasiparticle matrix element can be evaluated by standard methods of tensor operators and angular momentum recoupling[5,47] requiring us to know only the reduced matrix elements of the quasiparticle operators. These can be evaluated by expanding a particular component of the operator in question, say λ^{ℓ}_{0}, and the bra and ket in terms of

quasiparticle or ordinary particle creation and annihilation operators, and then applying the Wigner-Eckart theorem.

If the general expression for the eigenfunctions of H is written in its modified form (Section 4)

viz. $$N\{\ldots\}\prod_{i=1}^{n} M^{\lambda}_{(\pm x\pm y,}M^{\mu}_{\pm x\pm y}|\bar{0}\rangle$$

then it is clear that $A_o^{\ell_p}$ ($p \neq 2n+1$, $A = \lambda, \mu, \xi, \nu$) acts only on the $M^{\lambda}M^{\mu}$ product where x or y equals p. If we write $(\Gamma_A)_i$ as

$$(-1)^{r+1+\frac{1}{2}(1-(-1)^a)(\ell_y+\ell_x)}\tfrac{1}{2},$$

i.e. $\pm\frac{1}{2}$ or $\pm(-1)^{\ell_y+\ell_x}\tfrac{1}{2}$ if $A = \mu, \nu$ and r is an arbitrary integer, and similarly for $(\Gamma_B)_i$, with t replacing r (A,B are a pair as defined in Section 2) then we find

$$A_o^{\ell_p}|(\Gamma_A)_i(\Gamma_B)_i\rangle = (-1)^{\frac{1}{2}[r(1-(-1)^p)+p+\ell_p-(1-(-1)^a)(\ell_p-r-t-1)]}$$

$$\frac{1}{\sqrt{2}}\,|-(\Gamma_A)_i(\Gamma_B)_i\rangle,$$

$$p \neq 2n+1$$

if the states are properly normalised, and other quantum numbers have been suppressed as unimportant. Since the rest of the Γ vector has remained unchanged we have the

selection rule that $A_o^{\ell_p}$ acts only between $|\Delta_a^{\uparrow(\downarrow)}\Delta_b^A\rangle$ and $|\Delta_{a'}^{\uparrow(\downarrow)}\Delta_{b'}^A,\rangle$ which in turn implies that coupled products of the form $\frac{1}{2}(A^{\ell}A^{\ell'})^{(K)}_Q$ can act only between $|\Delta_a^{\uparrow(\downarrow)}\Delta_b^A\Delta_c^B\rangle$ and $|\Delta_a^{\uparrow(\downarrow)}\Delta_b^A\Delta_c^B\rangle$ while products of the form $\frac{1}{2}(A^{\ell}B^{\ell'})^{(K)}_Q$ can act only between $|\Delta_a^{\uparrow(\downarrow)}\Delta_b^A\Delta_c^B\rangle$ and $|\Delta_a^{\uparrow(\downarrow)}\Delta_b^A,\Delta_c^B,\rangle$.

As in Chapter 3 we can now write a general expression for the reduced matrix element for the particular case of maximum $L = L_M$ by noting under our separation of the duplicated L_M's that

$$|(\Delta_a^{\uparrow})(\Delta_b^{\lambda}\,\Gamma^{\lambda}\,L_M\text{-}L_M),(\Delta_c^{\mu}\,\Gamma^{\mu}\,L_ML_M)\rangle \;=\; N\prod_i^n M^{\lambda}M^{\mu}|\overline{0}\rangle$$

where the Δ and Γ are determined by the particular form of M. This gives us

$$\langle\Delta_{m'}^{\uparrow(\downarrow)}\Delta_{n'}^A\text{-}(\Gamma)_i^AL_M||A^{\ell_x}||\Delta_m^{\uparrow(\downarrow)}\Delta_n^A(\Gamma)_i^AL_M\rangle$$

$$= P(-1)^{\frac{p+\ell_p}{2}}\;\frac{[(2L_M-\ell_p)!(2L_M+\ell_p+1)!/2]^{\frac{1}{2}}}{(2L_M)!}\qquad (p \neq 2n+1)\quad \text{(IV-8)}$$

where $P = (-1)^{\frac{1}{2}[n(1-(-1)^p)+m(1-(-1)^a]}$ and m and n are used as before. For p odd the Δ^A label is not present. In this case we find, as in Chapter 3

$$\langle \Delta_m^{\uparrow(\downarrow)} L_M || A^{\ell_{2n+1}} || \Delta_{m'} \rangle = (-1)^{\frac{1}{2}[(1+(-1)^a)\ell_{2n+1}+(1+(-1)^m)\times} \times (\ell_{2n+1}+a)]$$

$$\frac{[(2L_M-\ell_{2n+1})!(2L_M+\ell_{2n+1}+1)!/2]^{\frac{1}{2}}}{(2L_M)!} \qquad \text{(IV-9)}$$

We note that these matrix elements can be both real and imaginary so the matrix element of a general operator will in general be complex. This perhaps unsatisfactory state of affairs is a natural consequence of the possible imaginary coefficients we have to take in order to form eigenfunctions of the H operators of the various groups. If we consider two quasiparticle states $|QP\rangle = \sum_i a_i |i\rangle$ and $|QP\rangle' = \sum_k b_k |k\rangle$, where the $|i\rangle$ and $|k\rangle$ are ordinary states and the a_i, b_k can be both real and imaginary, then if W is any operator and

$$W|i\rangle = \sum_j W_{ij}|j\rangle, \qquad \text{where } W_{ij} \text{ is real, then}$$

$$\langle QP|W|QP\rangle = \sum_{ijk} b_k^* a_i W_{ij}\langle k|j\rangle = \sum_{ij} b_j^* a_i W_{ij}$$

which is in general complex. It is not hard to see that if W is hermitian and $|QP\rangle = |QP\rangle'$ then the expectation value of W is real. We find that $W^{(kk)}(\ell_i \ell_j)$ has real matrix elements if $(-1)^{i+j} = (-1)^{\ell_i+\ell_j}$.

To conclude this section we shall evaluate the diagonal matrix element of $W^{(02)}_{00}(sd)$ of $(s+d)^N$ with the state $|(\Delta_1^\uparrow)(\Delta_1^\lambda \tfrac{3}{2}^\lambda)(\Delta_1^\mu \tfrac{3}{2}^\mu)L=3,M_L=3\rangle$. The Γ quantum numbers are not used as they are unnecessary for two orbitals. The only part of $W^{(02)}_{00}(sd)$ that we are interested in is $\frac{1}{2\sqrt{2}}(\lambda^0\lambda^2)^{(2)}_0 - (\mu^0\mu^2)^{(2)}_0$ as the rest vanishes by the selection rules above. Since

$$\langle \Delta_1^\uparrow \Delta_1^\lambda \tfrac{3}{2}||\lambda^0||\Delta_2\Delta_2^\lambda\rangle = i\sqrt{2} \qquad \langle \Delta_2^\uparrow \Delta_2^\lambda \tfrac{3}{2}||\lambda^2||\Delta_1^\uparrow\Delta_1^\lambda \tfrac{3}{2}\rangle = \sqrt{10}$$

$$\langle \Delta_1^\uparrow \Delta_1^\mu \tfrac{3}{2}||\mu^0||\Delta_2\Delta_2^\mu\rangle = i\sqrt{2} \qquad \langle \Delta_2^\uparrow \Delta_2^\mu \tfrac{3}{2}||\mu^2||\Delta_1^\uparrow\Delta_1^\mu \tfrac{3}{2}\rangle = -\sqrt{10}, \tag{IV-10}$$

then

$$\langle (\Delta_1)^\uparrow(\Delta_1^\lambda \tfrac{3}{2}^\lambda, \Delta_1^\mu \tfrac{3}{2}^\mu)L=3,M_L=3|W^{(02)}_{00}(sd)|(\Delta_1^\uparrow)(\Delta_1^\lambda \tfrac{3}{2}^\lambda, \Delta_1^\mu \tfrac{3}{2}^\mu) L=3,M_L=3\rangle$$

$$= + \frac{1}{2\sqrt{2}} \begin{pmatrix} 3 & 2 & 3 \\ -3 & 0 & 3 \end{pmatrix} 7\sqrt{5} \begin{Bmatrix} \frac{3}{2} & \frac{3}{2} & 0 \\ \frac{3}{2} & \frac{3}{2} & 2 \\ 3 & 3 & 2 \end{Bmatrix}$$

$$\begin{bmatrix} \langle \Delta_1^\uparrow \Delta_1^\lambda \tfrac{3}{2}||\lambda^0||\Delta_2^\uparrow\Delta_2^\lambda \tfrac{3}{2}\rangle\langle \Delta_2^\uparrow \Delta_2^\lambda \tfrac{3}{2}||\lambda^2||\Delta_1^\uparrow\Delta_1^\lambda \tfrac{3}{2}\rangle \\ -\langle \Delta_1^\uparrow \Delta_1^\mu \tfrac{3}{2}||\mu^0||\Delta_2^\uparrow\Delta_2^\mu \tfrac{3}{2}\rangle\langle \Delta_2^\uparrow \Delta_2^\mu \tfrac{3}{2}||\mu^2||\Delta_1^\uparrow\Delta_1^\mu \tfrac{3}{2}\rangle \end{bmatrix}$$

$$= i\sqrt{\frac{5}{14}}$$

8. Conclusions

In this Chapter I have examined the application of the quasiparticle formalism to mixed configurations. As would have been anticipated from the results of the last chapter, we obtain a remarkably rich classification scheme that permits the matrix elements of interactions to be calculated without the usual recourse to coefficients of fractional parentage but rather by the more common vector coupling methods. Compared with the previously treated case of equivalent electron orbitals there has, however, been a not unexpected increase in complexity. Recall, for instance, the care that must be taken over the precise form of the eigenfunctions of the Weyl operators (Section 4) and the complexity of the matrix elements (Section 6). Where many orbitals are involved the problem of handling the duplications arising in the decomposition of the spin representations under $R_\rho \rightarrow R_3$ will become increasingly severe, though of course the same holds for the conventional methods.

The quasi-formalism gives further insight into the mathematical structure of atomic shell theory and in this respect its study is valuable. The fact that the quasiparticle eigenfunctions involve linear combinations of eigenfunctions defined on different numbers of particles constitutes the fundamental weakness of the scheme from a

physical viewpoint. In the case of the angular parts of the wavefunction this is of no moment but in terms of the radial parts we certainly do not wish to assume their invariance with respect to the number of particles. This objection could of course be overcome by projecting out wavefunctions defined on a definite number of particles but only with an ensuing increase in complexity.

C H A P T E R V

RADIAL MATRIX ELEMENTS OF THE RADIAL-ANGULAR FACTORIZED HYDROGEN ATOM

1. Introduction

The selection rule, on hydrogenic radial integrals, discovered by Pasternack and Sternheimer[48], namely

$$\int_0^\infty \frac{R_{n\ell}R_{n\ell'}}{r^s}\, r^2 dr = 0 \qquad s = 2,3,\ldots|\ell-\ell'|+1$$

has stimulated recently at least two attempts to explain it group theoretically. That of Swamy, Kulkarni and Biedenharn[49] is based on the O(4) symmetry of the hydrogen atom and uses a complex recursive technique. Armstrong[9] approaches the problem more directly by showing that radial-like functions of two variables, r and τ, transform according to representations of the non-compact group O(2,1) and in this scheme, he shows that positive and negative powers of r have tensorial transformation properties. Armstrong's scheme however is unsatisfactory for two important reasons. Firstly his two variable functions of r and τ never complete coincide with true one variable radial functions of $\frac{r}{n}$ where n is the principal quantum number. As

one consequence of this no treatment of off diagonal matrix elements can be given. Secondly, Armstrong's radial-like functions and their associated O(2,1) group stand isolated from any encompassing group scheme such as the O(4,2) model of Barut and Kleinert[8]. Kleinert[52] has written a paper containing an excellent review of this model.

These difficulties are met in this paper by considering the hydrogen atom factorized into its radial (O(2,1)) and angular (O(3)) parts, according to the scheme $O(4,2) \supset O(3) \times O(2,1)$ of Barut and Kleinert[8,52]. Here the true radial wavefunctions of the variable $\frac{r}{n}$ transform according to a representation of the O(2,1) group (section 2) and it is shown that the quantity $r^k D_{n/n+q}$ for all positive and negative integer k, where D_a is a dilatation operator defined by $D_a f(x) = f(ax)$, is proportional to the q^{th} component of a tensor (Section 3). The Pasternack and Sternheimer selection rule follows naturally and since the Wigner-Eckart theorem is shown to hold (Section 4) calculation of the appropriate Clebsch-Gordan coefficients (Section 5) allows matrix elements to be calculated. Some progress is made on the difficult problem of off diagonal elements of r^k (Section 5).

2. The Group Scheme

The fifteen generators $L_{\mu\nu}$, $1 < \mu < \nu < 6$, of $O(4,2)$ are defined in terms of their action on the hydrogen atom wavefunction written in parabolic coordinates[8,52]. Their commutation relations are given by

$$[L_{\mu\nu}L_{\mu\lambda}] = ig_{\mu\mu}L_{\nu\lambda} \qquad g_{\alpha\alpha} = 1 \quad 1 < \alpha < 4, \qquad = -1 \quad 5 < \alpha < 6$$

A subgroup $O(3) \times O(2,1)$ can be formed with the $O(3)$ generators given by L_{12}, L_{23}, L_{13} and the $O(2,1)$ generators given by L_{45}, L_{46} and L_{56}. These last generators are formed into the linear combinations $K_{\pm} = L_{45} \mp iL_{46}$ and $K_0 = L_{56}$ to give the standard $O(2,1)$ commutation relations[50,51] of

$$[K_0K_{\pm}] = \pm K_{\pm} \qquad \text{and} \qquad [K_+K_-] = -2K_0$$

Consider now the entire hydrogen atom wave function

$$|n\ell m\rangle = R_{n\ell}(x_n)Y_{\ell m}(\theta\varphi)$$

where

$$R_{n\ell}(x_n) = N_{n\ell}\, e^{-x_n}\, (2x_n)^{\ell}\, L^{2\ell+1}_{n-\ell-1}(2x_n) \qquad (V\text{-}1)$$

$$N_{n\ell} = -(-1)^{n+\ell}\frac{2Z^{\frac{3}{2}}}{n^2}\left[\frac{(n-\ell-1)!}{(n+\ell)!}\right]^{\frac{1}{2}} \qquad x_n = \frac{Zr}{n}$$

and $Y_m^{\ell}(\theta\varphi)$ are the usual spherical harmonics. A Hilbert space is defined by the inner product

$$\int_0^{\infty} \int_{\Omega} R_{n'\ell'}(x_{n'}) Y_{\ell' m} \, x_{n'}^2 \, R_{n\ell}(x_n) Y_{\ell m} \, \frac{n'^2 n}{Z^3} \, dx_n \, d\Omega$$

$$= \delta(nn')\delta(\ell\ell') \qquad \text{(V-2)}$$

where $d\Omega = \sin\theta d\theta d\varphi$.

In the $O(4,2) \supset O(2,1) \times O(3)$ scheme of Barut and Kleinert[8] these wavefunctions for fixed m form a basis of a representation of O(2,1) since

$$K_{\pm}|n\ell m\rangle = [(n\mp\ell)(n\pm\ell\pm 1)]^{\frac{1}{2}}|n\pm 1 \; \ell m\rangle$$

$$\text{and} \quad K_0|n\ell m\rangle = n|n\ell m\rangle \qquad \text{(V-3)}$$

The representation has only a lower bound on the O(2) quantum number (equal to $\ell+1$) and is shown below to be unitary and irreducible. Equation (V-3) implies that the realization in this Hilbert space of the generators of O(2,1) is

$$K_{\pm} = \mp \left(\frac{n\pm 1}{n}\right) D_{\frac{n}{n\pm 1}} + \left(x_n \frac{\partial}{\partial x_n} \mp x_n \pm n + 1\right) \qquad \text{(V-4)}$$

and $K_0 = n$

where D_a is a dilatation operator defined such that $D_a f(r) = f(ar)$, which implies that

$$D_{\frac{n}{n'}} f(x_n) = f(x_{n'}).$$

If we form the Casimir invariant

$$G = K_0^2 - \tfrac{1}{2}(K_+K_- + K_-K_+)$$

we find that

$$\int_0^\infty \int_\Omega R_{n\ell} Y_{\ell m} x_n^2 G\, R_{n\ell} Y_{\ell m} \frac{n^3}{Z^3}\, dx_n = \langle n\ell m|G|n\ell m\rangle = \ell(\ell+1) \tag{V-5}$$

However, Barut and Fronsdal[51] show that the eigenvalues of G are of the form $\Phi(\Phi+1)$. If a representation is bounded below, its lower bound is $-\Phi$. If Φ is negative, the representation is unitary and labelled $D^+_{-\Phi}$. All this implies that the wavefunctions $|n\ell m\rangle$ for fixed m form a basis for the unitary irreducible representation $D^+_{\ell+1}$.

3. The Tensorial Properties of r^k

In this section, it is shown that the quantity

$$\frac{r^k}{(n+q)^{k-1}} D_{\frac{n}{n+q}} A^{\ell}_{\ell'}(\theta\varphi)$$

where q and k are integers, transforms as the qth component of an O(2,1) tensor operator, the associated representation depending upon the size of k relative to -2. Here $A^{\ell}_{\ell'}$ is an operator defined such that

$$A^{\ell}_{\ell'}(\theta\varphi)Y_{\ell m} = Y_{\ell' m} \qquad (V\text{-}6)$$

To be specific we can build $A^{\ell}_{\ell'}$ up as a power of products $A^{\ell}_{\ell+1}$ or $A^{\ell}_{\ell-1}$ where

$$A^{\ell}_{\ell+1} = \left[\frac{2\ell+3}{(\ell+1-m)(\ell+1+m)(2\ell+1)}\right]^{\frac{1}{2}}\{(\ell+\tfrac{1}{2})\cos\theta + \sin\theta\,\frac{d}{d\theta}\}$$

see for instance Infeld and Hull[53].

Consider

$$\langle n+q\pm1\ \ell m|[K_{\pm}, \frac{r^k}{(n+q)^{k-1}} D_{\frac{n}{n+q}}\ A^{\ell'}_{\ell}\ |n\ \ell' m\rangle$$

$$= \mp\int_0^{\infty}\int_{\Omega} R_{n+q\pm1\ell}Y_{\ell m}\, x^2_{n+q\pm1}\left\{\left(\frac{n+q\pm1}{n+q}\right) D_{\frac{n+q}{n+q\pm1}}\,(x_{n+q}\frac{\partial}{\partial x_{n+q}}\right.$$

$$\mp x_{n+q} \pm n \pm q + 1)(n+q)\, x^{k+2}_{n+q} D_{\frac{n}{n+q}}$$

$$\left. - (n+q\pm1)x^{k+2}_{n+q\pm1} D_{\frac{n\pm1}{n+q\pm1}} \times \left(\frac{n\pm1}{n}\right) D_{\frac{n}{n\pm1}}(x_n\frac{\partial}{\partial x_n} \mp x_n \pm n + 1)\right\}$$

$$\times A^{\ell'}_{\ell} R_{n\ell'} Y_{\ell' m}\ \frac{(n+q\pm1)^2 n}{Z^{3+k}}\, dx_n\, d\Omega$$

$$= \int_0^{\infty}\int_{\Omega} R_{n+q\pm1}(n+q\pm1)\, x^{k+2}_{n+q\pm1}\{(x_{n+q\pm1}\frac{\partial}{\partial x_{n+q\pm1}} \mp x_{n+q\pm1} + k$$

$$+ 2 \pm n \pm q + 1) - (x_{n+q\pm1}\frac{\partial}{\partial x_{n+q\pm1}} \mp x_{n+q\pm1} \pm n + 1)\}$$

$$D_{\frac{n}{n+q\pm 1}} A_{\ell}^{\ell'} R_{n\ell'} Y_{\ell' m} \frac{(n+q\pm 1)^2 n}{Z^{3+k}} dx_n \, d\Omega$$

$$= \mp (k+2\pm q) \int_0^\infty \int_\Omega R_{n+q\pm 1} Y_{\ell m} (n+q\pm 1) x_{n+q\pm 1}^{k+2} D_{\frac{n}{n+q\pm 1}}$$

$$\times A_{\ell}^{\ell'} R_{n\ell'} Y_{\ell' m} \frac{(n+q\pm 1)^2 n}{Z^3} dx_n \, d\Omega$$

$$= \mp (k+2\pm q) \langle n+q\pm 1 \; \ell m | \frac{r^k}{(n+q\pm 1)^{k-1}} D_{\frac{n}{n+q\pm 1}} A_{\ell}^{\ell'} | n\ell' m \rangle \qquad (V-7)$$

We see then that if $k+2 < 0$

$$\left[K_{\pm}, \frac{r^k}{(n\mp k+2)^{k-1}} D_{\frac{n}{n\mp k\mp 2}} A_{\ell}^{\ell'} \right] = 0$$

i.e. $k+2 < q < -k-2$ while if $k+2 > 0$

$$\left[K_{\mp}, \frac{r^k}{(n\pm k\pm 2)^{k-1}} D_{\frac{n}{n\pm k\pm 2}} A_{\ell}^{\ell'} \right] = 0$$

Hence if $k < -2$ we have a representation of finite dimension equal to $-2k-3$ labelled D_{-k-2}, while if $k > -2$, the representation is infinite dimensional and reducible, but not fully reducible, for while the spaces $q > k+2$ and $q < -k-2$ are invariant under the group operations, the space $-k-1 < q < k+1$ is not. This representation will be

labelled as D'_{k+1}. Both of these representations are non-unitary since the eigenvalues of $K_{\pm}K_{\mp}$ are not positive definite[51]. This means we are free to normalize our tensor operators in an arbitrary manner, and a particular choice is made in Section 5.

4. The Wigner-Eckart Theorem

A well-known method for proving the Wigner-Eckart theorem for O(3) (see for instance Messiah[54]) sets up recursion relations between different matrix elements of the q^{th} and $(q\pm1)^{th}$ components of an O(3) tensor operator and shows that these are identical to the recursion relations for the corresponding O(3) Clebsch-Gordan coefficients. This implies that Clebsch-Gordan coefficient and matrix element are proportional, the proportionality constant being the reduced matrix element. This proof in fact requires only that if $J_i|\ell m\rangle = a_i|\ell m_i\rangle$ then $[J_i T^{\ell}_m] = a_i T^{\ell}_{m_i}$, where J_i is an O(3) generator, and T^{ℓ}_m an O(3) tensor operator, and that the states being coupled up to be orthonormal.

In the O(2,1) case we first write the states corresponding to the representations D_{-k-2} and D'_{k+1} as $|kq\rangle$, where the use of k and q distinguishes them from the states $|n\ell\rangle$ of $D^{+}_{\ell+1}$, and the corresponding tensor operator

as

$$N_{kq} \frac{r^k}{(n+q)^{k-1}} \; D_{\frac{n}{n+q}} \; A_{\ell}^{\ell'}$$

where N_{kq} is some arbitrary normalization. We have then that

$$K_{\pm}|kq\rangle = \pm(k+2\pm q) \frac{N_{kq}}{N_{kq\pm1}} |kq\pm1\rangle$$

and

$$[K_{\pm}, T^k_q] = \pm(k+2\pm q) \frac{N_{kq}}{N_{kq\pm1}} T^k_{q\pm1}$$

K_0 in both cases gives an eigenvalue of q.

It therefore follows that since the states $|n\ell\rangle$ are orthonormal, the Wigner-Eckart theorem holds, and we can write

$$\langle \ell n m | T^k_q | \ell' n' m \rangle = \langle \ell || T^k || \ell' \rangle \, C^{\ell' k \ell}_{n' qn} \qquad \text{(V-8)}$$

where $C^{\ell' k \ell}_{n' qn}$ is an O(2,1) Clebsch-Gordan coefficient coupling the states of $D^+_{\ell'+1}$ with the states of either D_{-k-2} or D'_{k+1}, normalised as above, to the states of $D^+_{\ell+1}$, while $\langle \ell || T^k || \ell' \rangle$ is the reduced matrix element and is independent of n, n' and q.

5. The Racah Algebra

In this section the Clebsch-Gordan coefficients appropriate to the representations we are considering are derived. The Pasternack and Sternheimer selection rule drops out naturally during the analysis. The reduced matrix elements of T^k are derived, allowing the diagonal matrix elements of r^k to be calculated. A brief discussion of the off-diagonal elements of r^k concludes the chapter.

The most direct means of deriving the Clebsch-Gordan coefficients, namely that of coupling two representations and the contragradient of a third to an invariant is perhaps most well-known in Bargmann's work[55], but is due to van der Waerden[56]. Barut and Fronsdal[51] have used this technique to derive some O(2,1) Clebsch-Gordan coefficients for unitary representations. This method has the advantage of not requiring an explicit form for the arbitrary normalization of the states of non-unitary representations.

To apply this technique we must first realize the representations in terms of multi-spinors $N_{ab}\xi^a\eta^b$ where N_{ab} is a normalization constant and the quantity (ξ,η) called a spinor, forms a basis for the fundamental irreducible representation of O(2,1). In this realization

$$K_0 = \tfrac{1}{2}\left(\xi\frac{\partial}{\partial\xi} - \eta\frac{\partial}{\partial\eta}\right) \qquad (V\text{-}9)$$

$$K_+ = \xi\frac{\partial}{\partial\eta} \qquad K_- = -\eta\frac{\partial}{\partial\xi} \tag{V-9}$$

So $K_0 N_{ab}\xi^a\eta^b = \frac{1}{2}(a-b)N\xi^a\eta^b$

and $G\ N_{ab}\xi^a\eta^b = \frac{1}{4}(a-b)(a-b+2)N_{ab}\xi^a\eta^b$.

Hence, if the eigenvalues of G and K_0 are respectively $\Phi(\Phi+1)$ and m then the states are represented by $N_{ab}\xi^{\Phi+m}\eta^{\Phi-m}$ where N_{ab} is shown by Barut and Fronsdal to be equal to $\left[\frac{(m-1-\Phi)!}{(m+\Phi)!}\right]^{\frac{1}{2}}$ for the unitary representation D^+_Φ. As remarked above N_{ab} is arbitrary for non-unitary representations.

We now form an invariant coupling of two representations and a contragradient representation defined as

$$\langle\Phi_m| = N_m^{-1}\ \xi^{\Phi-m}\ \eta^{\Phi+m} \tag{V-10}$$

giving

$$I = \sum_{m_1 m_2 m_3} C^{\Phi_1\ \Phi_2\ \Phi_3}_{m_1\ m_2\ m_3} N_1\ \xi_1^{\Phi_1+m_1}\ \eta_1^{\Phi_1-m_1}\ N_2\ \xi_2^{\Phi_2+m_2}$$

$$\eta_2^{\Phi_2-m_2}\ N_3^{-1}\ \xi_3^{\Phi_3-m_3}\ \eta_3^{\Phi_3+m_3} \tag{V-11}$$

where I is an invariant in the space of the polynomials of $\prod_i \xi_i^{a_i}\ \eta_i^{b_i}$. However, since the representation matrices are unimodular the only invariants in this space are the three determinants

$$\delta_1 = \xi_2\eta_3 - \xi_3\eta_2, \quad \delta_2 = \xi_3\eta_1 - \xi_1\eta_3, \quad \delta_3 = \xi_1\eta_2 - \xi_2\eta_1$$

and every mononomial in these, see Bargmann[55]. Hence

$$\delta_1^{k_1}\delta_2^{k_2}\delta_3^{k_3} = \sum_{m_1 m_2 m_3} C^{\Phi_1\ \Phi_2\ \Phi_3}_{m_1\ m_2\ m_3} N_1\, \xi_1^{\Phi_1+m_1}\, \eta_1^{\Phi_1-m_1}$$

$$\times N_2\, \xi_2^{\Phi_2+m_2}\, \eta_2^{\Phi_2-m_2}\, N_3\, \xi_3^{\Phi_3-m_3}\, \eta_3^{\Phi_3+m_3} \qquad (V\text{-}12)$$

This implies

$$k_2+k_3 = 2\Phi_1, \qquad k_3+k_1 = 2\Phi_2, \qquad k_2+k_1 = 2\Phi_3 \qquad (V\text{-}13)$$

or equivalently

$$k_1 = \Phi_2+\Phi_3-\Phi_1, \qquad k_2 = \Phi_3+\Phi_1-\Phi_2, \qquad k_3 = \Phi_1+\Phi_2-\Phi_3 \qquad (V\text{-}14)$$

We now note that

$$(\xi_a\eta_b - \xi_b\eta_a)^n = \sum_{s\geq 0} \binom{n}{s} (\xi_a\eta_b)^s(-\xi_b\eta_a)^{n-s}$$

$$\text{or} \quad \sum_{s\geq 0} \binom{n}{s} (\xi_a\eta_b)^{n-s}(-\xi_b\eta_a)^s$$

for all positive and negative integer n, so by comparing coefficients we have

$$N_1 N_2 N_3^{-1} \, C^{\Phi_1\ \Phi_2\ \Phi_3}_{m_1\ m_2\ m_3} = \sum_{pqr} (-1)^{p+q+r} \binom{k_1}{p} \binom{k_2}{q} \binom{k_3}{r} \qquad (V\text{-}15)$$

Consider first $k < -2$. In this case the representation D_{Φ_2} is finite-dimensional, while $D^+_{\Phi_1}$ and $D^+_{\Phi_3}$ are infinite-dimensional. Inspection of (V-12) shows that this requires k_1 and k_3 to be positive and k_2 negative. Taking these constraints and substituting

$$\Phi_1 = -\ell-1, \qquad \Phi_3 = -\ell'-1, \qquad \Phi_2 = -k-2 = s-2$$

into (V-14) gives the Pasternack and Sternheimer selection rule, namely

$$2 \leq s \leq |\ell-\ell'|+1 \qquad (V\text{-}16)$$

gives a vanishing matrix element.

To case (V-15) into a useful form we put $p = z$. From (V-12) we see that $p+q = \Phi_3-m_3$ and $p+r = \Phi_2+m_2$ so that (V-15) becomes

$$N_1 N_2 N_3^{-1} \, C^{\ell\ \ k\ \ \ell'}_{n\ n'-n\ n'} = \sum_z (-)^{k+\ell'+1+n+z}$$

$$\times \binom{\ell-\ell'-k-2}{z} \binom{k-\ell-\ell'}{1-\ell-k+n'+z} \binom{\ell'-\ell-k-2}{\ell'-\ell-n'+n+z} \quad (k < -2) \qquad (V\text{-}17)$$

This formula is quite adequate as it stands (after substituting for N) but it is of interest to note with

Armstrong, that it can be cast into a form that shows that this O(2,1) Clebsch-Gordan coefficient is in fact equal, to within a phase, to the O(3) Clebsch-Gordan coefficients.

To do this, equation (V-17) is expanded in factorial notation (remembering that $k-\ell-\ell'$ is negative) and identities I and II derived in Appendix I are applied giving

$$A\left[\frac{(\ell+n)!(\ell'+n')!}{(k-q)!(k+q)!(n-\ell-1)!(n'-\ell'-1)!}\right]^{\frac{1}{2}}$$

$$\times \sum_t (-1)^t \frac{(k+n-\ell'-1-t)!(k+n'+\ell-t)!}{t!(k-\ell'+\ell-t)!(n+\ell-t)!(n'-\ell'-1-t)!}$$

where A contains unimportant constant terms. N_2 has been chosen as $[(-k-2-q)!(-k-2+q)!]^{-\frac{1}{2}}$ which implies that $K_{\pm}|kq\rangle = \mp[(k\mp q)(k\pm q\pm 1)]^{\frac{1}{2}}|kq\pm 1\rangle$. If the Clebsch-Gordan coefficients are now renormalized to satisfy the orthonormality condition

$$\sum_{qn} C^{\ell\ k\ \ell'}_{n\ q\ n'} C^{\ell\ k\ \ell''}_{n\ q\ n''} (-1)^{\ell+\ell'+q} = \delta(\ell'\ell'')\delta(n'n'') \qquad \text{(V-18)}$$

This condition has been derived by Armstrong, and an independent derivation for a more general case is given in Chapter VI (VI-12).

$$C^{\ell\ k\ \ell'}_{n\ q\ n'} = (-1)^{k+q}\left[\frac{(\ell'-\ell-k-2)!(\ell+\ell'+k+2)!(\ell-\ell'-k-2)!}{(\ell+\ell'-k-1)!}\right]^{\frac{1}{2}}$$

$$\times\left[\frac{(n'-\ell'-1)!(\ell'+n')!(-k-2-q)!(2\ell'+1)}{(-k-2+q)!(\ell+n)!(n-\ell-1)!}\right]^{\frac{1}{2}}$$

$$\times\ \sum_t (-1)^{t+k+q}\binom{\ell'-n'+t}{-k-2-q}\binom{k+n'+\ell-t}{\ell'+n'}\binom{\ell+n}{t}$$

$$= a\ \langle kq, \ell n \mid \ell' n' \rangle \qquad \text{(V-19)}$$

where a=1 if $\ell-\ell'$ is even and -i if $\ell-\ell'$ is odd.

We consider now the case of $k \geq -2$. In this case it is convenient to put r = z giving

$$N_1 N_2 N_3^{-1}\ C^{\ell\ \ k\ \ \ell'}_{n\ n'-n\ n'} = \sum_z (-1)^{\ell'+1+n'+z}$$

$$\times\binom{\ell-\ell'+k+1}{\ell-\ell'-n'+n+z}\binom{-2-\ell-\ell'-k-1}{-1-\ell'-k-1+n+z}\binom{\ell'-\ell+k+1}{z} \qquad \text{(V-20)}$$

The power of this technique is illustrated here, for Armstrong, using the recursive technique of Racah[57] derives these particular Clebsch-Gordan coefficients for q = n'-n equal to zero only.

Since in this case Φ_2 is positive, we cannot have both k_1 and k_3 negative, so if we assume $\ell \geq \ell'$ we have two possibilities, namely both $\ell-\ell'+k+1$ and $\ell'-\ell+k+1$ positive

or $\ell-\ell'+k+1$ positive and $\ell'-\ell+k+1$ negative. Since q = 0 is the case of most interest, we will consider the case of k+q positive; thus the first possibility allows equation (V-19) to be transformed exactly as was equation (V-20) to give

$$\frac{(\ell-\ell'+k+2)!(\ell'+n')!}{(k+1+q)!}$$

$$\sum_t \frac{(k+n'-\ell-t)!}{(k+2+\ell-n'+t)!(n'+\ell'-t)!(n'-\ell'-1-t)!(n-\ell-1-t)!t!} \qquad \text{(V-21)}$$

where each N_i has been put equal to one. The second case transforms via identity III to the same expression.

Equation (V-20) is also proportional to the corresponding O(3) Clebsch-Gordan coefficient since it is of the same form as that taken by equation (V-5) after the application of identity I.

The reduced matrix elements can be derived from first principles by considering the matrix element

$$\langle \ell+1\ \ell' m | T^k | \ell+1\ \ell m \rangle = C^{\ell}_{\ell+1\ 0\ \ell+1}{}^{k\ \ell'} \langle \ell' || T^k || \ell \rangle$$

$$= \int_0^\infty \int_\Omega R_{\ell+1\ \ell'} Y_{\ell' m} \frac{r^{k+2}}{(\ell+1)^{k-1}} A^{\ell}_{\ell'} R_{\ell+1\ \ell} Y_{\ell m}\, dr d\Omega \quad (\ell > \ell') \qquad \text{(V-22)}$$

The integral through Ω is one, and since $L_0^{2\ell+1}$ is a

constant, equation (V-22) becomes a sum of integrals of the form

$$\int_0^\infty e^{-ax}\, x^b dx \;=\; \frac{b!}{a^{b+1}}$$

provided that $b > -1$, i.e. provided that $\ell+\ell'+k+2 > 0$. The integral evaluates to

$$\tfrac{1}{2}\,\frac{1}{(2Z)^k}\left[\frac{1}{(2\ell+1)!(\ell+\ell'+1)!(\ell-\ell')!}\right]^{\frac{1}{2}}\frac{(\ell+\ell'+k+2)!(\ell-\ell'+k+1)!}{(k+1)!} \qquad k > -2$$

or

$$\tfrac{1}{2}\,\frac{1}{(2Z)^k}\left[\frac{1}{(2\ell+1)!(\ell+\ell'+1)!(\ell-\ell')!}\right]^{\frac{1}{2}}\frac{(-k-2)!(\ell+\ell'+k+2)!}{(\ell'-\ell-k-2)!} \qquad k < -2$$

However, since

$$C^{\ell\ k\ \ell'}_{\ell+1\ 0\ \ell+1} \;=\; (-1)^{k+q}\left[\frac{(2\ell'+1)}{2\ell+1}\right]^{\frac{1}{2}} C^{\ell'\ k\ \ell}_{\ell+1\ 0\ \ell+1}$$

$$= \frac{(\ell-\ell'+k+1)}{(\ell-\ell')!(k+1)!}\left[\frac{(\ell+\ell'+1)!}{(\ell-\ell')!(2\ell+1)}\right]^{\frac{1}{2}} \qquad k > -2$$

or $$\left[\frac{(2\ell'+1)(\ell-\ell'-k-2)!(\ell+\ell'+k+2)!(\ell+\ell'-k-1)!}{(2\ell+1)!(\ell'-\ell)!(\ell'-\ell-k-2)!(\ell+\ell'+1)!}\right]^{\frac{1}{2}} \qquad k < -2$$

we have

$$\langle \ell' \,||T^k||\, \ell\rangle \;=\; \tfrac{1}{2}\,\frac{1}{(2Z)^k}\,\frac{(\ell+\ell'+k+2)!(\ell-\ell')!}{(\ell+\ell'+1)!} \qquad k > -2$$

or $\frac{1}{2}\frac{1}{(2Z)^k}\left[\frac{(\ell+\ell'+k+2)!}{(\ell'-\ell-k-2)!(\ell-\ell'-k-2)!(\ell+\ell'-k-1)!(2\ell'+1)}\right]^{\frac{1}{2}}$

Since $D_{n/n} = 1$ and the integral through Ω is one, T^k is proportional to a matrix element of r^k, diagonal in n, namely

$$\int_0^\infty R_n\, r^k R_{n\ell'} r^2 dr = \langle n\ell m|r^k|n\ell' m\rangle$$

$$= n^{k-1}\langle n\ell m|T^k|n\ell' m\rangle \qquad k > -2$$

$$= n^{k-1}(-k-2)!\langle n\ell m|T^k|n\ell' m\rangle \qquad k < -2$$

(V-23)

Off diagonal elements of r^k however are much harder to deal with. Placing a complete set of states in the expression

$$\langle n_p\ell_p m|N^k_{n_p n_q} r^k\, D_{n_q/n_p}\cdot D_{n_p/n_q} A^{\ell_q}_{\ell_p}|n_q\ell_q m\rangle$$

(where $N^k_{n_p n_q}$ is the normalization required to make $r^k D_{n_q/n_p} A^{\ell_q}_{\ell_p}$ into a tensor operator) will not do because $r^k D_{n_q/n_p} A^{\ell_q}_{\ell_p}$ is a tensor operator between the states $|n_p\ell_p m\rangle$ and $|n_q\ell_q m\rangle$ only. A formal solution to this problem can be given by inverting the infinite matrix formed by putting a complete set of states in the expression

$\langle n_p \ell_p m | T^k_{n_p - n_r} | n_r \ell_r m \rangle$. Thus

$$\langle n_p \ell_p m | T^k_{n_p - n_r} | n_r \ell_r m \rangle \equiv \langle n_p \ell_p m | N^k_{n_p n_r} r^k D_{n_r/n_p} A^{\ell_r}_{\ell_p} | n_r \ell_r m \rangle$$

$$= \sum_{n_q} \langle n_p \ell_p m | r^k A^{\ell_r}_{\ell_p} | n_q \ell_r m \rangle \langle n_q \ell_r m | N^k_{n_p n_r} D_{n_r/n_p} | n_r \ell_r m \rangle$$

since D_{n_r/n_p} is diagonal in ℓ and m[8,52].

So

$$\langle n_p \ell_p m | T^k_{n_p - n_r} | n_r \ell_r m \rangle = \sum_{n_q} A_{qr} \int_0^\infty R_{n_p \ell_p} r^k R_{n_q \ell_r} r^2 dr$$

where A is the infinite matrix whose elements are

$$A_{qr} = \langle n_q \ell_r m | N^k_{n_p n_r} D_{n_r/n_p} | n_r \ell_r m \rangle .$$

This is, in principle, invertible to give

$$\int_0^\infty R_{n_p \ell_p} r^k R_{n_q \ell_1} r^2 dr = \sum_{n_q} A^{-1}_{qr} \langle n_p \ell_p m | T^k_{n_p - n_q} | n_q \ell_r m \rangle$$

6. Conclusions

In this chapter I have shown how to circumvent some of the difficulties encountered when one uses the "natural" group scheme for the hydrogen atom, namely $O(4,2) \supset O(3) \times O(2,1)$ to explain the selection rule of Pasternack and Sternheimer and to derive corresponding matrix elements. A complete treatment of off diagonal matrix elements is not yet available since in this group scheme it is $r^k D_{n/n'}$ and not r^k, as might be hoped, that is proportional to a tensor operator.

C H A P T E R V I

AN O(2,1) × O(3) SOLUTION TO A GENERALIZED QUANTUM MECHANICAL KEPLER PROBLEM

1. Introduction

The method of the last chapter is used on a more general differential equation directly related to the generalised Kepler equation of Infeld and Hull[53]. This allows a unified treatment of all quantum mechanical Kepler problems in an O(2,1) × O(3) scheme, since the Schrodinger, Klein-Gordan and Dirac hydrogen atoms, the latter diagonalised in the usual k scheme (see for instance Bethe and Salpeter[58]) or the S scheme of Biedenharn[59], are special cases of this equation.

As in the Schrodinger case if ν is the O(2) quantum number of the radial wave-function in the basis $O(2,1) \supset O(2)$ then $r^k D_{\nu/\nu+q}$, k,q integers, is proportional to the q^{th} component of a tensor operator. Here D_a is a dilatation operator defined such that $D_a f(x) = f(ax)$. A generalised Pasternack and Sternheimer selection rule exists and matrix elements diagonal in the O(2) quantum number can be derived group theoretically.

Crubellier and Feneuille[60], have used the Infeld and Hull generalised Kepler equation to generalise Armstrong's[9]

O(2,1) treatment of the non-relativistic hydrogen atom to the k Dirac atom. As is explained in Chapter V, our method differs in that it follows the O(4,2) scheme of Barut and Kleinert in using dilatation operators and one variable radial wave functions.

2. Group Structure of the Generalised Kepler Equation

Consider the equation

$$\left(\nabla^2 - \frac{(\lambda-\ell)(\ell+\lambda+1)}{\rho^2} + \frac{2Z}{\rho} - \frac{Z^2}{\nu^2}\right)u(\rho\theta\varphi) = 0 \qquad \text{(VI-1)}$$

λ here is a monotonic function of ℓ, where ℓ and $\nu-\lambda$ are integers. Z is the charge on the nucleus. This separates in the usual manner giving the solution

$$u = R^{\lambda}_{\nu}(\rho)Y^{\ell}_{m}(\theta\varphi)$$

where $Y^{\ell}_{m}(\theta\varphi)$ is a spherical harmonic and $R^{\lambda}_{\nu}(\rho)$ satisfies the radial equation

$$\left(\frac{d^2}{d\rho^2} + \frac{2}{\rho}\frac{d}{d\rho} + \frac{2Z}{\rho} - \frac{Z^2}{\nu^2} - \frac{\lambda(\lambda+1)}{\rho^2}\right)R^{\lambda}_{\nu} = 0 \qquad \text{(VI-2)}$$

which is apart from minor variations the generalised Kepler equation of Infeld and Hull[53]. A solution to (VI-2) is

$$R^{\lambda}_{\nu} = N_{\lambda\nu}\, e^{-Z\rho/N} \left(\frac{2Z\rho}{\nu}\right)^{\lambda} L^{2\lambda+1}_{\nu-\lambda-1}\left(\frac{2Z\rho}{\nu}\right) \qquad \text{(VI-3)}$$

where $L^{2\lambda+1}_{\nu-\lambda-1}\left(\frac{2Z\rho}{\nu}\right)$ is a generalised Laguerre polynomial defined by

$$L^a_b(x) = \sum_{n=0}^{b} \frac{\Gamma(a+b+1)(-x)^n}{n!(b-n)!\Gamma(a+n+1)}$$

We have $$\int_0^\infty R^\lambda_\nu R^\lambda_{\nu'} \rho^2 d\rho = \delta(\nu\nu') \qquad \text{(VI-4)}$$

which requires

$$N_{\lambda\nu} = \frac{2}{\nu^2}\left[\frac{Z^3(\nu-\lambda-1)!}{\Gamma(\nu+\lambda+1)}\right]^{\frac{1}{2}}$$

If we now take the quantities

$$K_\pm = \mp\left(\frac{\nu\pm1}{\nu}\right) D_{\nu/\nu\pm1}\left(x_\nu\, \partial/\partial x_\nu \mp x_\nu \pm \nu + 1\right) \qquad \text{(VI-5)}$$

and $K_0 = \nu$

under the inner product

$$\int_0^\infty \int_\Omega R^\lambda_\nu Y^\ell_m\, x_\nu^2\, R^{\lambda'}_{\nu'}\, Y^{\ell'}_m\, x_{\nu'}\, \frac{\nu^2\nu'}{Z^3}\, dx_{\nu'}\, d\Omega = \delta(\nu\nu')\delta(\ell\ell')$$

$$= \delta(\nu\nu')\delta(\ell\ell')\delta(\lambda\lambda') \qquad \text{(VI-6)}$$

since λ is a monotonic function of ℓ. Here

$$x_\nu = \frac{Z\rho}{\nu} \quad \text{and} \quad d\Omega = \sin\theta d\theta d\varphi$$

As in Chapter V $D_{\nu/\nu\pm1}$ is a dilatation operator defined such that $D_a f(\rho) = f(a\rho)$, which implies that

$$D_{\nu/\nu'}\, f(x_\nu) = f(x_{\nu'})$$

This gives

$$K_\pm R^\lambda_\nu = [(\nu \mp \lambda)(\nu \pm \lambda \pm 1)]^{\frac{1}{2}} R^\lambda_{\nu\pm1}$$

$$K_0 R^\lambda_\nu = \nu R^\lambda_\nu$$

and

$$\int_0^\infty \int_\Omega R^\lambda_\nu Y^\ell_m x^2_\nu [K_+ K_-] R^\lambda_\nu Y^\ell_m \frac{\nu^3}{Z^3}\, dx_\nu d\Omega$$

$$= -\int_0^\infty \int_\Omega R^\lambda_\nu Y^\ell_m x^2_\nu \left\{ D_{\nu-1/\nu}(x_{\nu-1}\, \partial/\partial x_{\nu-1} - x_{\nu-1} + \nu) \right.$$

$$\cdot D_{\nu/\nu-1}\,(x_\nu\, \partial/\partial x_\nu + x_\nu - \nu + 1) - D_{\nu+1/\nu}(x_{\nu+1}\, \partial/\partial x_{\nu+1} + x_{\nu+1} - \nu)$$

$$\left. \cdot D_{\nu/\nu+1}(x_\nu\, \partial/\partial x_\nu - x_\nu + \nu + 1) \right\} R^\lambda_\nu Y^\ell_m \frac{\nu^3}{Z^3}\, dx_\nu d\Omega$$

$$= \int_0^\infty \int_\Omega R^\lambda_\nu Y^\ell_m x^2_\nu (-2K_0) R^\lambda_\nu Y^\ell_m \frac{\nu^3}{Z^3}\, dx_\nu d\Omega$$

Similarly $[K_0 K_\pm] = \pm K_\pm$.

Hence as in Chapter V, since the Y^ℓ_m form a basis for a representation of $O(3)$, the wave functions $R^\lambda_\nu Y^\ell_m$ for fixed m form the basis for a representation of the group $O(2,1) \times O(3)$. Following Chapter V, we find the eigenvalues of the Casimir invariant

$$G = K_0^2 - \tfrac{1}{2}(K_+ K_- + K_- K_+)$$

to be $\lambda(\lambda+1)$, and hence the wave functions $R^{\lambda}_{\nu}Y^{\ell}_{m}$ for fixed m form a basis for the representation $D^{+}_{\lambda+1}$ of O(2,1) and $\mathcal{D}^{\ell}$ of O(3).

Note that equation (VI-2) is in fact equivalent to $GR^{\lambda}_{\nu} = \lambda(\lambda+1)R^{\lambda}_{\nu}$ and hence is very similar to a type B Infeld and Hull factorisation[53], with $K_{\pm}$ acting as the step up - step down operators.

Four special cases are considered by specifying λ and ρ. They are

(1) Schrodinger hydrogen atom $\rho=r$, $\lambda=\ell$

(2) Klein-Gordan "hydrogen atom" $\rho=r$

$$\lambda=-\tfrac{1}{2}+[(\ell+\tfrac{1}{2})^2-Z^2\alpha^2]^{\frac{1}{2}}$$

(3) k Dirac hydrogen atom $\rho=ar$ where $a = \frac{\mu\varepsilon\alpha}{\hbar}$,

μ mass of nucleus and

$$\varepsilon = \left[1 + \frac{\alpha^2Z^2}{(n+\lambda)^2}\right]^{-\frac{1}{2}}, \quad \lambda = [k^2-\alpha^2Z^2]^{\frac{1}{2}}$$

(4) Biedenharn's[59] S Dirac hydrogen atom. In this case we have two iterated second order equations and $\rho = r$

$$\lambda = +(k^2-Z^2\alpha^2)^{\frac{1}{2}} - \tfrac{1}{2} + \tfrac{1}{2}\,\mathrm{sgn}(k).$$

The representation structures hence derived are in agreement with those given by Bacry and Richard[61], Barut and Bornzin[62] and Lanik[63].

3. Tensor Operators and the Racah Algebra

Having established our formalism the extension of Chapter V to this more general case is straightforward. First we consider the commutation relations of the O(2,1) generators with the quantity $\frac{\rho^k}{(\nu+q)^{k-1}} D_{\nu/\nu+q} A^{\ell}_{\ell'}(\theta\varphi)$, k and q integers, where

$$A^{\ell}_{\ell'}(\theta\varphi) Y^{\ell}_{m} = Y^{\ell'}_{m}$$

and find that it transforms according to the q^{th} component of a tensor operator whose representation is of finite dimension equal to $-2k-3$ if $k < -2$ and is labelled D_{-k-2} and of infinite dimension and reducible but not fully reducible if $k > -2$. This representation is labelled D'_{k+1}. Both of these representations are non-unitary since the eigenvalues of $K_+ - K_-$ are not positive definite[51].

As in Chapter V the Wigner-Eckart Theorem holds so

$$\langle \lambda \nu m | T^k_q | \lambda' \nu' m \rangle = \langle \lambda | | T^k | | \lambda' \rangle C^{\lambda' k \lambda}_{\nu' q \nu}$$

where $C^{\lambda' k \lambda}_{\nu' q \nu}$ is an O(2,1) Clebsch-Gordan coefficient. In Chapter V the representations were characterised by integers only; however the derivation of the Clebsch-Gordan coefficients in this case is unchanged except for the replacement of factorials by gamma functions at the appropriate places. Binomial identities used in their

derivation are still applicable since the addition theorem for binomial coefficients, namely

$$\sum_p \binom{k_1}{p}\binom{k_2}{r-p} = \binom{k_1+k_2}{r}$$

where $$\binom{a}{b} = \frac{\Gamma(a+1)}{\Gamma(b+1)\Gamma(a-b+1)}$$

holds for all values of k_1 and k_2.

We recall from Chapter V that the technique for deriving Clebsch-Gordan coefficients due to van der Waerden[56] and Bargmann[55] requires the representation states be realised by normalised multispinors $N_{ab}\xi^a\eta^b$. We then form an invariant coupling of two representations and a contragradient representation giving equation (V-12), namely

$$\delta_1^{k_1}\delta_2^{k_2}\delta_3^{k_3} = \sum_{m_1m_2m_3} C^{\Phi_1\Phi_2\Phi_3}_{m_1m_2m_3} N_1\,\xi_1^{\Phi_1+m_1}\,\eta_1^{\Phi_1-m_1} \qquad \text{(VI-6)}$$

$$\times N_2\,\xi_2^{\Phi_2+m_2}\,\eta_2^{\Phi_2-m_2}\,N_3\,\xi_3^{\Phi_3-m_3}\,\eta_3^{\Phi_3+m_3}$$

Here the δ_i are the three determinantal invariants

$$\delta_1 = \xi_2\eta_3-\xi_3\eta_2, \qquad \delta_2 = \xi_3\eta_1-\xi_1\eta_3, \qquad \delta_3 = \xi_1\eta_2-\xi_2\eta_1.$$

This implies

$$k_2+k_3 = 2\Phi_1, \qquad k_3+k_1 = 2\Phi_2, \qquad k_2+k_3 = 2\Phi_3 \tag{VI-7}$$

or equivalently

$$k_1 = \Phi_2+\Phi_3-\Phi_1, \quad k_2 = \Phi_3+\Phi_1-\Phi_2, \quad k_3 = \Phi_1+\Phi_2-\Phi_3 \tag{VI-8}$$

Expanding the left hand side of (VI-6) gives

$$\sum_{pqr} \binom{k_1}{p}\binom{k_2}{q}\binom{k_3}{r}(-1)^{k_1-p+q+r}\,\xi_1^{k_3-r+q}\,\eta_1^{k_2-q+r}\,\xi_2^{p+r} \times \eta_2^{k_1+k_3-p-r}\,\xi_3^{k_2+k_1-p-q}\,\eta_3^{p+q} \tag{VI-9}$$

In order that the correct representations are coupled we require k_1 and k_3 to be positive integers. This means that ξ_1, ξ_2 and ξ_3 are bounded below and η_2 is bounded above as required. Then by (VI-7) Φ_2 is a positive integer. The selection rule for negative k follows from (VI-8)

$$\Phi_1 + \Phi_2 - \Phi_3 = k_1 \geq 0$$

$$\Phi_2 + \Phi_3 - \Phi_1 = k_3 \geq 0 \quad \text{and} \quad \Phi_2 \geq 0$$

implies $\quad 0 \leq \Phi_2 \leq |\Phi_1-\Phi_3|$

Substituting

$$\Phi_1 = -\lambda-1, \qquad \Phi_3 = -\lambda'-1, \qquad \Phi_2 = -k-2 = s-2$$

gives

$$2 \leq s \leq |\lambda-\lambda'|+1$$

Comparing coefficients between (VI-6) and (VI-9) now gives the unnormalised Clebsch-Gordan coefficients. To normalize an orthogonality condition is required. This is derived by closer consideration of the direct product state $|\lambda\nu;kq\rangle$ where the state $|kq\rangle$ corresponds to the tensor $D_{\nu/\nu\pm1}A^{\ell}_{\ell'}$. The ℓ quantum numbers have been omitted as being unimportant. The set of states $|\lambda\nu\rangle$ form a basis for the unitary representation $D^{+}_{\lambda+1}$ so in this basis $K_{\pm}{}^{+} = K_{\mp}$ under the inner product $\langle\lambda'\nu'|\lambda\nu\rangle = \delta_{\lambda\lambda'}\delta_{\nu\nu'}$. However, the set $|kq\rangle$ does not form a unitary representation, so if we demand that $K_{\pm}{}^{+} = K_{\mp}$ in the direct product space we must define the inner product in this basis to be

$$\langle k'q'|kq\rangle = (-1)^{q}\delta(qq').$$

This is so since

$$\langle k'q'|K_{\pm}kq\rangle = \mp\,[(k\mp q)(k\pm q\pm1)]^{\frac{1}{2}}\langle k'q'|kq\rangle \qquad \text{(VI-10)}$$

from Chapter V, section 5.

So (VI-10) equals

$$\mp\,(-1)^{q}[(k\mp q)(k\pm q\pm1)]^{\frac{1}{2}}$$

$$= \langle K_{\pm}k'q'|kq\rangle.$$

i.e. $\quad K_{\pm}^{+} = K_{\mp}^{-}.$

Now if $|\lambda\nu\rangle = \sum_{\nu' q} C^{\lambda' k \lambda}_{\nu' q \nu} |\lambda'\ \nu'; kq\rangle$

taking the inner product with $\langle kq;\ \lambda''\ \nu''|$ gives as the required orthogonality condition

$$\sum_{\nu q} C^{\lambda k \lambda'}_{\nu q \nu'}\ C^{*}{}^{\lambda k \lambda''}_{\nu q \nu''}(-1)^{q} = \delta(\lambda'\lambda'')\delta(\nu'\nu'') \qquad \text{(VI-12)}$$

Finally then

$$C^{\lambda k \lambda'}_{\nu q \nu'} = (-1)^{k+q}\left[\frac{\Gamma(\lambda'-\lambda-k-1)\,\Gamma(\lambda+\lambda'+k+3)\,\Gamma(\lambda-\lambda'-k-1)}{\Gamma(\lambda+\lambda'-k)}\right]^{\frac{1}{2}}$$

$$\times\left[\frac{\Gamma(\nu'-\lambda')\,\Gamma(\nu'+\lambda')\,\Gamma(2\nu'+2)(-k-2-q)!}{\Gamma(\nu+\lambda+1)\,\Gamma(\nu-\lambda)(-k-2+q)!}\right]^{\frac{1}{2}}$$

$$\times \sum_{t} (-1)^{t+k+q}\binom{\lambda'-\nu'+t}{-k-2-q}\binom{k+\nu'+\lambda-t}{\nu'+\lambda'}\binom{\lambda+\nu}{t} \quad k > -2. \qquad \text{(VI-13a)}$$

$$C^{\lambda k \lambda'}_{\nu q \nu'} = \frac{\Gamma(\lambda-\lambda'+k+3)\,\Gamma(\lambda'+\nu'+1)}{(k+1+q)!}$$

$$\times \sum_{t} \frac{\Gamma(k+\nu'-\lambda-t+1)}{\Gamma(k+3+\lambda-\nu'+t)\,\Gamma(\lambda'+\nu'-t+1)\,\Gamma(\nu'-\lambda'-t)\,\Gamma(\nu-\lambda-t)\,t!}$$

$$k < -2 \qquad k+q > 0 \qquad \text{(VI-13b)}$$

In the second case $k+q < 0$ has not been considered as the case $q = 0$ is of most interest.

4. Matrix Elements

To complete this Chapter the reduced matrix elements for the generalised Kepler problem are derived. This is done by considering the matrix element

$$\langle \lambda' \lambda+1 | T_0^k | \lambda \lambda+1 \rangle = C^{\lambda}_{\lambda+1\ 0\ \lambda+1}{}^{k\ \ \lambda'} \langle \lambda' || T^k || \lambda \rangle \qquad (\lambda > \lambda')$$

Since $L_0^{2\ell+1}$ is a constant the integral becomes a sum of integrals of the form

$$\int_0^{\infty} e^{-ax} x^b dx = \frac{\Gamma(b+1)}{a^{b+1}}$$

provided that $b > -1$, i.e. provided that $\lambda+\lambda'+k+2 > -1$. Substituting for

$$C^{\lambda}_{\lambda+1\ 0\ \lambda+1}{}^{k\ \ \lambda'}$$

from (VI-13) gives

$$\langle \lambda' || T^k || \lambda \rangle = \tfrac{1}{2} \frac{1}{(2Z)^k} \frac{\Gamma(\lambda+\lambda'+k+3)\Gamma(\lambda-\lambda'-1)}{\Gamma(\lambda+\lambda')} \qquad k < -2 \qquad \text{(VI-14a)}$$

$$\text{or} \quad \tfrac{1}{2} \frac{1}{(2Z)^k} \left[\frac{\Gamma(\lambda+\lambda'+k+3)}{\Gamma(\lambda'-\lambda-k-1)\Gamma(\lambda-\lambda'-k-1)\Gamma(\lambda+\lambda'-k)\Gamma(2\ell'+2)} \right]^{\frac{1}{2}} \qquad \text{(VI-14b)}$$

To illustrate this technique we shall derive a matrix element for the k Dirac hydrogen atom important in the theory of hyperfine structure[64]. Using the notation of Bethe and Salpeter[58] we note first that

$$\chi_1 = \left(\frac{\varepsilon a}{2Z}\right)^{\frac{1}{2}} \frac{1}{2\gamma} \{(\gamma_2+\gamma_1)(\varepsilon k-\gamma)^{\frac{1}{2}} \rho R_\nu^{\gamma-1} + (\gamma_2-\gamma_1)(\varepsilon k+\gamma)^{\frac{1}{2}} \rho R_\nu^{\gamma}\}$$

and

$$\chi_2 = \left(\frac{\varepsilon a}{2Z}\right)^{\frac{1}{2}} \frac{1}{2\gamma} \{(\gamma_2-\gamma_1)(\varepsilon k-\gamma)^{\frac{1}{2}} \rho R_\nu^{\gamma-1} + (\gamma_2+\gamma_1)(\varepsilon k+\gamma)^{\frac{1}{2}} \rho R_\nu^{\gamma}\}$$

where $\gamma_1 = (k-\alpha Z)^{\frac{1}{2}}$, $\gamma_2 = (k+\alpha Z)^{\frac{1}{2}}$, $\lambda = \gamma = \gamma_1\gamma_2$.

Consider now the matrix element $\int_0^\infty \frac{\chi_1\chi_2 dr}{r^2}$. This equals

$$\frac{\varepsilon a^2}{8Z^2\nu^3\gamma^2} \{(\gamma_2^2-\gamma_1^2)(\varepsilon k-\gamma)\int_0^\infty R_\nu^{\gamma-1} \frac{\nu^3}{\rho^2} R_\nu^{\gamma-1} \rho^2 d\rho$$

$$+ (\gamma_2^2-\gamma_1^2)(\varepsilon k+\gamma) \int_0^\infty R_\nu^{\gamma} \frac{\nu^3}{\rho^2} R_\nu^{\gamma} \rho^2 d\rho\}$$

since by the selection rule the terms containing different γ vanish. Substituting from equation (VI-12) and (VI-13) gives finally

$$\int_0^\infty \frac{\chi_1\chi_2 dr}{r^2} = \frac{\varepsilon a^2 \alpha Z}{\nu^3} \left(\frac{2\varepsilon k-1}{\gamma(4\gamma^2-1)}\right)$$

in agreement with Crubellier and Feneuille.[60] In the same

way a second matrix element important in hyperfine structure evaluates as

$$\int_0^\infty \frac{(\chi_1^2+\chi_2^2)dr}{r^3} = \frac{\varepsilon a^3 k}{2\gamma^3\nu^3}\left\{\frac{(\varepsilon k-\gamma)}{(\gamma-\frac{1}{2})(\gamma-1)} + \frac{(\varepsilon k+\gamma)}{(\gamma+\frac{1}{2})(\gamma+1)}\right\}$$

$$+ \frac{2a^3\varepsilon\alpha Z}{\gamma^2\nu^3(4\gamma^2-1)}\{(\varepsilon^2k^2-\gamma^2)(\nu^2-\gamma^2)\}^{\frac{1}{2}}$$

5. Conclusions

As in Chapter V a formal solution for off diagonal matrix elements can be given. However, considerable refinement of the technique would seem to be necessary before a closed formula could be found for this difficult problem. Further progress would now appear to lie in the direction of the many electron problem which awaits some approximate dynamical group structure to describe complex atoms.

Generalising the Kepler problem in a different sense it would be interesting to see if the model proposed by Barut and Bornzin[62] for dyons does not also have a tensor operator with a Pasternack and Sternheimer selection rule.

C H A P T E R V I I

GENERAL CONCLUSIONS

Section I: The detailed structure of the theory of representations of compact groups, in particular the formulas for coupling coefficients, has received much attention in the last decade (see bibliography to Louck's[4] review paper) especially in the pioneering works of Biedenharn and co-workers[18], and Moshinsky and co-workers[17] in generalising the Wigner calculus to the unitary canonical chain. However, beyond a few special cases little is known about the representation theory of non-compact groups. As larger groups become used in elementary particle physics and possibly atomic spectroscopy, this situation may change.

Section II: The highly non-physical aspects of the quasi-particle scheme are compensated by a rich classificatory scheme and no cfp's in the operator calculus. Additionally Armstrong and Judd[12] have shown that the quasiparticle formalism can be used to explain many of the more obscure selection rules found otherwise by inspection in Nielson and Koster[25].

The next step in this field of the application of continuous groups to atomic spectroscopy appears to be some attempt to solve the many-electron problem entirely - that is both angular and radial parts by the use of non-compact groups. This could be done by finding some approximate dynamical group for the atom as a whole. Armstrong has suggested a re-examination of Layzer's[65] approach with this in mind. Another approach would be to attempt a solvable many-body problem group theoretically, such as the delta function interparticle interaction[66], and use the lessons learnt as a guide to more realistic problems. In either case the atomic spectroscopists would do well to keep abreast with developments in elementary particle theory in the hope that a similar cross fertilization of ideas such as the hydrogen atom and hadron O(4,2) model of Barut and co-workers may occur again.

APPENDIX I

SOME COMBINATORIAL IDENTITIES

The addition theorem for binomial coefficients, namely

$$\sum_s \binom{x}{s}\binom{y}{z-s} = \binom{x+y}{s}$$

gives

(a) $$\frac{a!}{b!c!} = \sum_s \frac{(a-b)!(a-c)!}{(a-b-s)!(a-c-s)!(b+c-a+s)!s!}$$

if x and y are positive;

(b) $$\sum_s (-1)^s \frac{(a-s)!}{s!(b-s)!(c-s)!} = (-1)^c \frac{(a-c)!(b+c-a-1)!}{b!c!(b-a-1)!}$$

if y is negative and $b > a \geq c > 0$;

or $$\frac{(a-b)!(a-c)!}{b!c!(a-b-c)!}$$

if y is negative and $a \geq b > 0$, $a \geq c > 0$;

(c) $$\frac{a!}{b!c!} = \sum_s (-1)^s \frac{(a-c)!(s-a+b-1)!}{(b-a-1)!\ s!(a-c-s)!(b-a+c+s)!}$$

if x is negative.

$$\text{I.} \quad \sum_t \frac{(a-t)!}{(b-t)!(c-t)!(d-t)!(e+t)!t!}$$

$$= \sum_{t,s} \frac{(a-b)!(a-c)!}{(a-b-s)!(a-c-s)!(b+c-a+s-t)!s!(d-t)!(e+t)!t!}$$

by (a)

$$= \frac{(a-b)!(a-c)!}{d!(d+e)!} \sum_s \frac{(b+c+d+e-a+s)!}{(b+c+e-a+s)!(b+c-a+s)!(a-b-s)!(a-c-s)!s!}$$

also by (a).

Equivalently

$$\sum_s \frac{(a+s)!}{(b+s)!(c+s)!(d-s)!(e-s)!s!}$$

$$= \frac{(a-b)!(a-c)!}{d!\ e!} \sum_t \frac{(d+e+c-t)!}{(a-b-t)!(e+c-t)!(d+c-t)!(b-c+t)!t!}$$

$$\text{II.} \quad \sum_s (-1)^s \frac{(a-s)!(b-s)!}{s!(c-s)!(d-s)!(e-s)!}$$

$$= \sum_{s,t} \frac{(-1)^s(a-c)!(a-d)!(b-s)!}{t!(a-c-t)!(a-d-t)!(c+d-a-s+t)!(e-s)!s!}$$

by (a);

$$= \sum_t \frac{(a-c)!(a-d)!(b-e)!(b+a-c-d-t)!}{e!(a-c-t)!t!(a-d-t)!(c+d-a+t)!(b+a-c-d-e-t)!}$$

by (b).

III. $\sum_t \frac{(a-t)!}{(b-t)!(c-t)!(d-t)!(e+t)!t!}$ a-b negative

$$= \frac{(a-c)!}{d!(d+e)!(b-a-1)!} \sum_s \frac{(-1)^s(b-a+c+d+e+s)!(b-a-1+s)!}{(b-a+c+e+s)!s!(a-c-s)!(b-a+c+s)!}$$

by (c) and (a).

Equivalently

$$\sum_s \frac{(-a)^s(a+s)!(b+s)!}{(c+s)!(d+s)!(e-s)!s!} = \frac{(a-c)!(a-d)!b!}{e!}$$

$$\sum_t \frac{(e+d-b-1-t)!}{(e+d-t)!(c-d+t)!(d-b-1-t)!(a-c-t)!}$$

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PUBLICATIONS

A large part of this thesis has either been published or accepted for publication in the Journal of Mathematical Physics, namely Chapters III and IV which were done with Professor Wybourne, and Chapter I. Chapter V has been accepted for publication while Chapter VI has been submitted.

In detail:

Chapter I: "Second Quantized Atomic Wavefunctions with Definite Unitary and Rotational Symmetry", J. Math. Phys. 11, 2781 (1970).

Chapter III: "Quasiparticle Formalism and Atomic Shell Theory", J. Math. Phys. 10, 2149 (1969).

Chapter IV: "Quasiparticle Formalism and Atomic Shell Theory II. Mixed Configurations", J. Math. Phys. 11, 1288 (1970).

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